96810 [redacted], [redacted] please

Access DB# _____

SEARCH REQUEST FORM

Scientific and Technical Information Center

Requester's Full Name: SABIHA QAZI (STIC) Examiner #: 74141 Date: 6/10/03
Art Unit: 1616 Phone Number 30 5-3910 Serial Number: 09/864,000
Mail Box and Bldg/Room Location: 2019 3B07 Results Format Preferred (circle): PAPER DISK E-MAIL

If more than one search is submitted, please prioritize searches in order of need.

****

Please provide a detailed statement of the search topic, and describe as specifically as possible the subject matter to be searched. Include the elected species or structures, keywords, synonyms, acronyms, and registry numbers, and combine with the concept or utility of the invention. Define any terms that may have a special meaning. Give examples or relevant citations, authors, etc, if known. Please attach a copy of the cover sheet, pertinent claims, and abstract.

Title of Invention: New 7-alpha-17-alpha bis-alkylated testosterone.

Inventors (please provide full names): Arwed Cleve et al.

Earliest Priority Filing Date: 371 of PCT/EP99/10355, 12/23/1999

**For Sequence Searches Only* Please include all pertinent information (parent, child, divisional, or issued patent numbers) along with the appropriate serial number.*

Please search for testosterone derivatives 6/10/03

of Cl 1. Elected Sp. is Compd No 80 elected

Please note a double bond at 4-5 and a carbonyl at 3 position & 7 position is always substituted.

Please see attached Structures

Thanks

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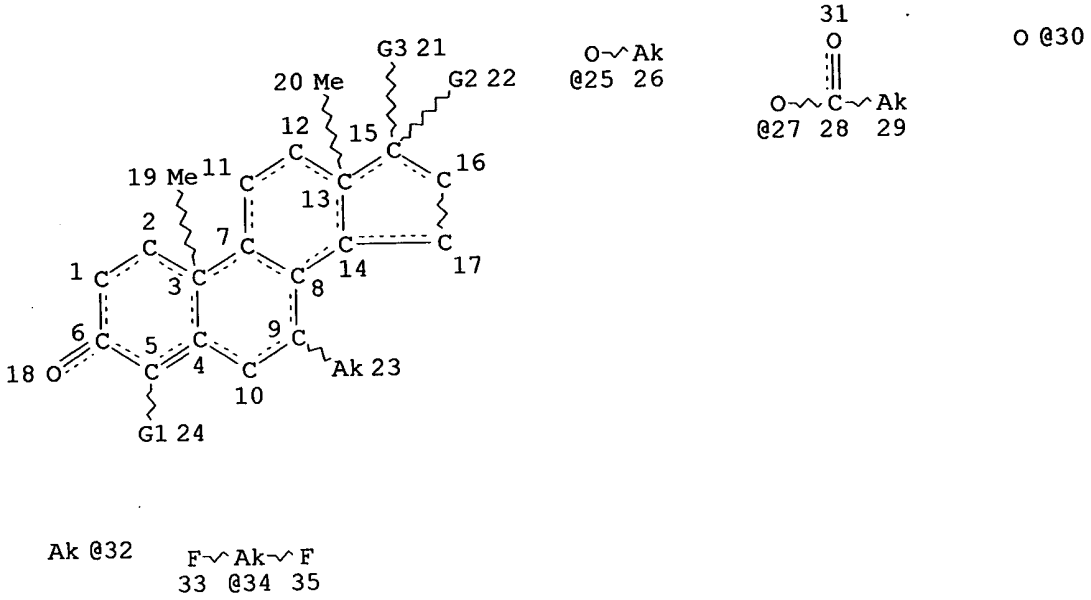
STAFF USE ONLY	Type of Search		Vendors and cost where applicable	
Searcher:	NA Sequence (#)		STN	288.78
Searcher Phone #:	AA Sequence (#)		Dialog	
Searcher Location:	Structure (#)	1	Questel/Orbit	
Date Searcher Picked Up:	6/20		Dr.Link	
Date Completed:	6/21		Lexis/Nexis	
Searcher Prep & Review Time:	20		Sequence Systems	
Clerical Prep Time:			WWW/Internet	
Online Time:	11		Other (specify)	

PTO-1590 (8-01)

=> d que
L1 STR



VAR G1=H/30/25/27
VAR G2=32/34
VAR G3=30/25/27
NODE ATTRIBUTES:
CONNECT IS E2 RC AT 16
CONNECT IS E2 RC AT 17
CONNECT IS E1 RC AT 26
CONNECT IS E1 RC AT 29
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CONNECT IS E1 RC AT 32
DEFAULT MLEVEL IS ATOM
GGCAT IS LOC AT 32
GGCAT IS LOC SAT AT 34
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS M6 C AT 23

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 35

STEREO ATTRIBUTES: NONE
L3 119 SEA FILE=REGISTRY SSS FUL L1
L4 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L3

=> d ibib abs hitstr

L4 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2003 ACS
ACCESSION NUMBER: 2000:442168 HCAPLUS
DOCUMENT NUMBER: 133:74180
TITLE: Preparation of new testosterone derivatives and their

use in the long-term therapy of androgen-dependent illnesses

INVENTOR(S): Cleve, Arwed; Sauer, Gerhard; Huwe, Christoph; Parczyk, Karsten; Hoffmann, Jens; Schneider, Martin

PATENT ASSIGNEE(S): Schering A.-G., Germany

SOURCE: Ger. Offen., 41 pp.
CODEN: GWXXBX

DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19860719	A1	20000629	DE 1998-19860719	19981223
WO 2000039148	A1	20000706	WO 1999-EP10355	19991223
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1140972	A1	20011010	EP 1999-967003	19991223
EP 1140972	B1	20030305		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
JP 2002533471	T2	20021008	JP 2000-591059	19991223
AT 233782	E	20030315	AT 1999-967003	19991223
NO 2001003168	A	20010622	NO 2001-3168	20010622

PRIORITY APPLN. INFO.: DE 1998-19860719 A 19981223
WO 1999-EP10355 W 19991223

OTHER SOURCE(S): MARPAT 133:74180

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

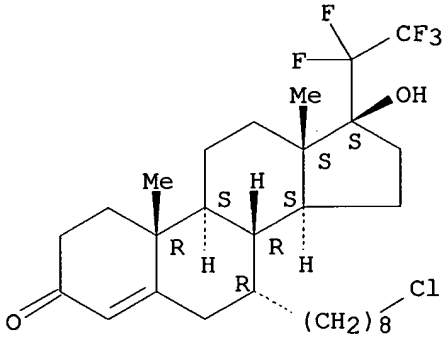
AB The available invention concerns new 7.alpha.,17.alpha.,17.beta.-substituted testosterone derivs. I [A = C6-13-alkylene; B = O, S(O)p, NY, NYCO, NYSO2, OSO2, OSiMe2, SCO, connection between A and CC; p = 0, 1, 2; Y = H, C1-8-alkyl, or together with CC a connection between A and CD, CC a connection between B and CD, or together with B a connection between A and CD, C1-6-alkyl, (un)substituted phenylene, vinyl, C1-4-alkoxy; C1-4-alkoxycarbonyl, bis(C1-4-alkoxycarbonyl)methyl] and their use as pure anti-androgens in the long-term therapy of androgen-dependent illnesses, in particular for the long-term anti-androgen therapy of the prostate carcinomas. Thus, antiandrogen II was prepd. from 17.alpha.-methyl-3-oxoandrosta-4,6-dien-17.beta.-yl acetate (III). II was tested for antiproliferation activity against against human prostate carcinoma LNCaP [IC50 = 40 nM].

IT **278603-67-1P 278603-68-2P 278603-72-8P 278603-92-2P 278603-97-7P 278604-10-7P**

278604-11-8P 278604-12-9P 278604-20-9P
278604-21-0P 278604-22-1P 278604-23-2P
278604-24-3P 278604-25-4P 278604-26-5P
278604-27-6P 278604-28-7P 278604-30-1P
278604-31-2P 278604-32-3P 278604-33-4P
278604-35-6P 278604-36-7P 278604-38-9P
278604-39-0P 278604-40-3P 278604-41-4P
278604-42-5P 278604-43-6P 278604-46-9P
278604-52-7P 278604-57-2P 278604-60-7P
278604-66-3P 278604-79-8P 278604-80-1P
278605-00-8P 278605-02-0P 278605-05-3P
278605-09-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses)
(prepn. of new testosterone derivs. and their use in the long-term therapy of androgen-dependent illnesses)

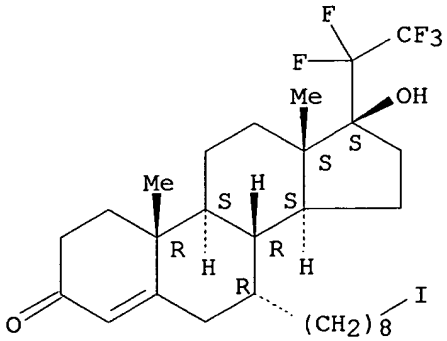
RN 278603-67-1 HCAPLUS
CN Pregn-4-en-3-one, 7-(8-chlorooctyl)-20,20,21,21,21-pentafluoro-17-hydroxy-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



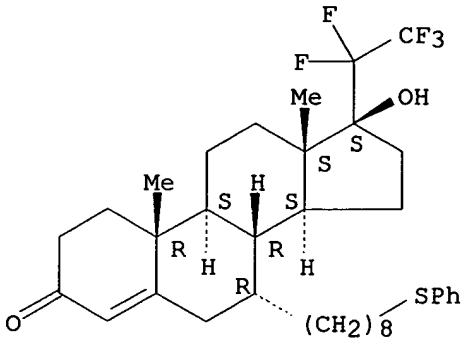
RN 278603-68-2 HCAPLUS
CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-(8-iodooctyl)-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



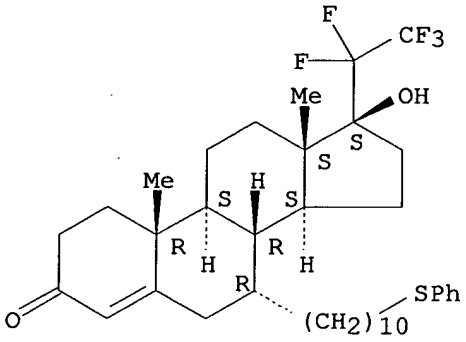
RN 278603-72-8 HCAPLUS
CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[8-(phenylthio)octyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



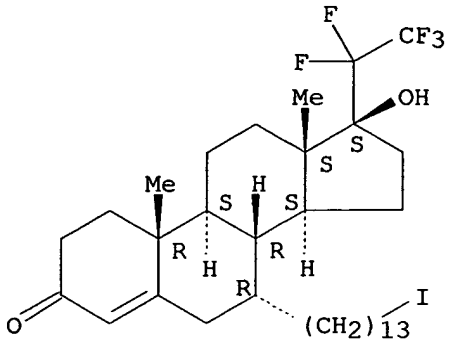
RN 278603-92-2 HCAPLUS
CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[10-(phenylthio)decyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



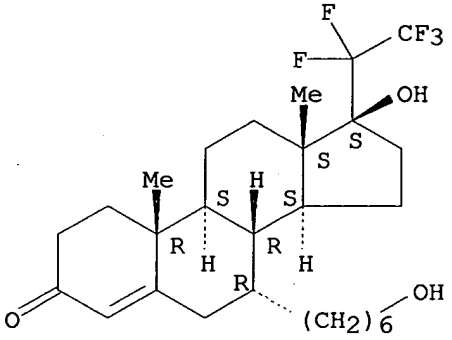
RN 278603-97-7 HCAPLUS
CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-(13-iodotridecyl)-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



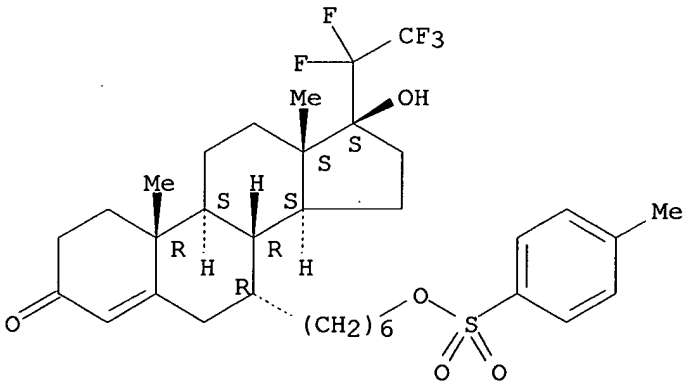
RN 278604-10-7 HCAPLUS
CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-(6-hydroxyhexyl)-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 278604-11-8 HCAPLUS
CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[6-[[(4-methylphenyl)sulfonyl]oxy]hexyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

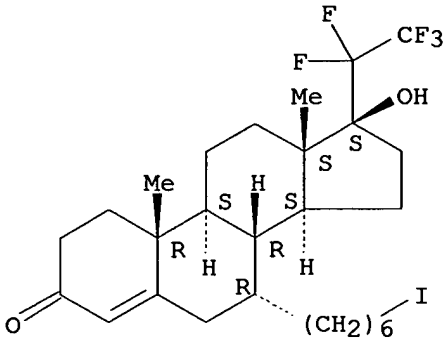
Absolute stereochemistry.



RN 278604-12-9 HCAPLUS

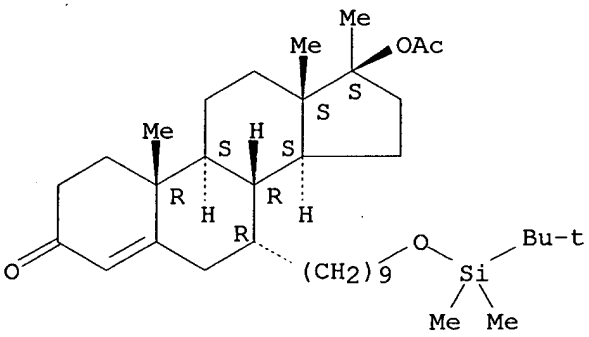
CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-(6-iodohexyl)-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



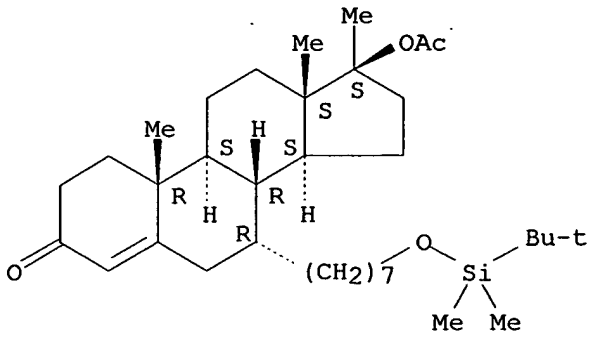
RN 278604-20-9 HCAPLUS
CN Androst-4-en-3-one, 17-(acetyloxy)-7-[9-[[(1,1-dimethylethyl)dimethylsilyl]oxy]nonyl]-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



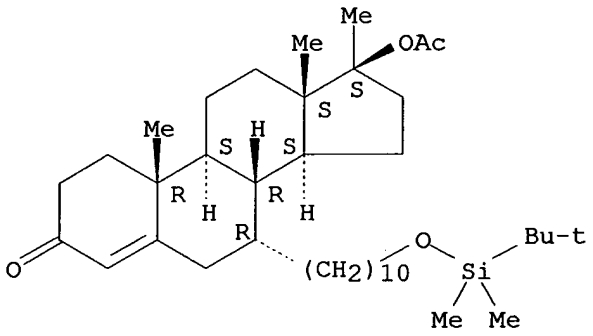
RN 278604-21-0 HCAPLUS
CN Androst-4-en-3-one, 17-(acetyloxy)-7-[7-[[(1,1-dimethylethyl)dimethylsilyl]oxy]heptyl]-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



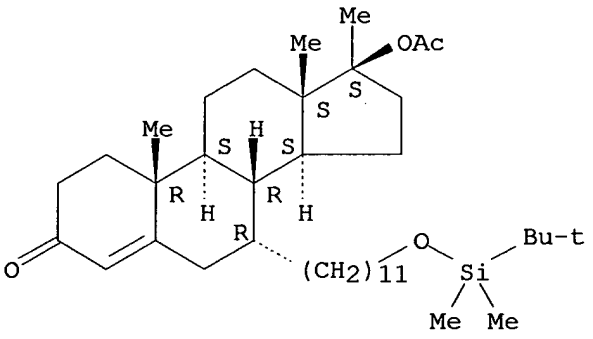
RN 278604-22-1 HCAPLUS
CN Androst-4-en-3-one, 17-(acetyloxy)-7-[10-[[(1,1-dimethylethyl)dimethylsilyl]oxy]decyl]-17-methyl-, (7.alpha.,17.beta.)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 278604-23-2 HCAPLUS
CN Androst-4-en-3-one, 17-(acetyloxy)-7-[11-[[(1,1-dimethylethyl)dimethylsilyl]oxy]undecyl]-17-methyl-, (7.alpha.,17.beta.)-(9CI) (CA INDEX NAME)

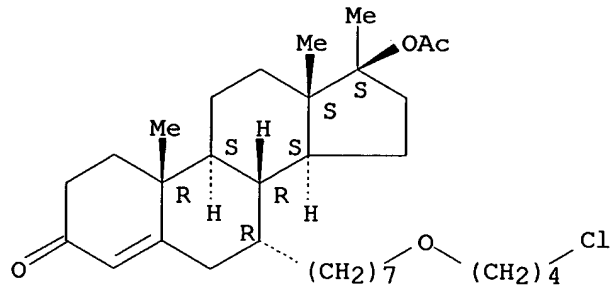
Absolute stereochemistry.



RN 278604-24-3 HCAPLUS

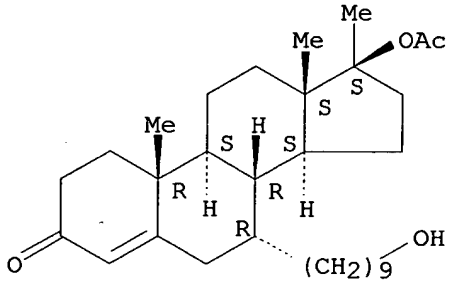
CN Androst-4-en-3-one, 17-(acetyloxy)-7-[7-(4-chlorobutoxy)heptyl]-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



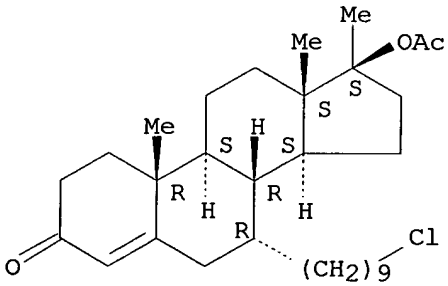
RN 278604-25-4 HCAPLUS
CN Androst-4-en-3-one, 17-(acetyloxy)-7-(9-hydroxynonyl)-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



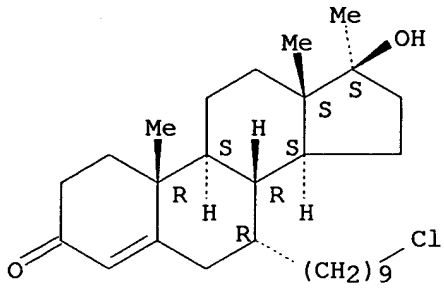
RN 278604-26-5 HCAPLUS
CN Androst-4-en-3-one, 17-(acetyloxy)-7-(9-chlorononyl)-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



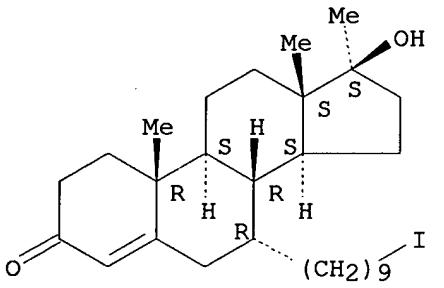
RN 278604-27-6 HCAPLUS
CN Androst-4-en-3-one, 7-(9-chlorononyl)-17-hydroxy-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



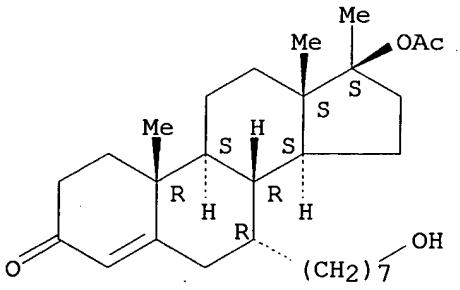
RN 278604-28-7 HCAPLUS
CN Androst-4-en-3-one, 17-hydroxy-7-(9-iodononyl)-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



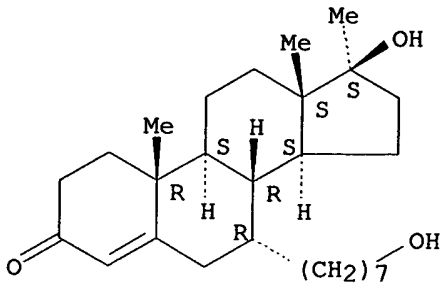
RN 278604-30-1 HCAPLUS
CN Androst-4-en-3-one, 17-(acetyloxy)-7-(7-hydroxyheptyl)-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 278604-31-2 HCAPLUS
CN Androst-4-en-3-one, 17-hydroxy-7-(7-hydroxyheptyl)-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 278604-32-3 HCAPLUS
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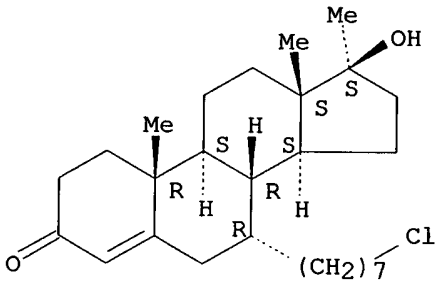
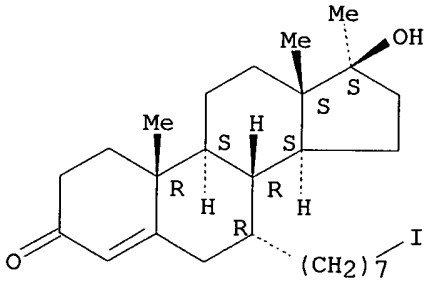
Absolute stereochemistry.



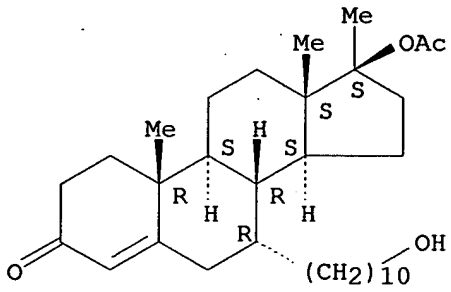
RN 278604-33-4 HCAPLUS
CN Androst-4-en-3-one, 17-hydroxy-7-(7-iodoheptyl)-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



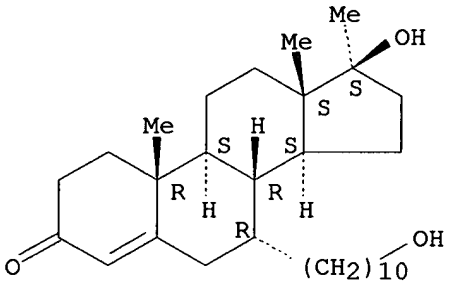
RN 278604-35-6 HCAPLUS
CN Androst-4-en-3-one, 17-(acetyloxy)-7-(10-hydroxydecyl)-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



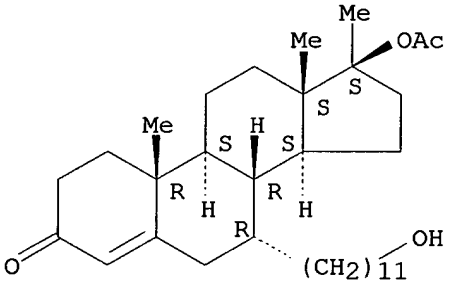
RN 278604-36-7 HCAPLUS
CN Androst-4-en-3-one, 17-hydroxy-7-(10-hydroxydecyl)-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



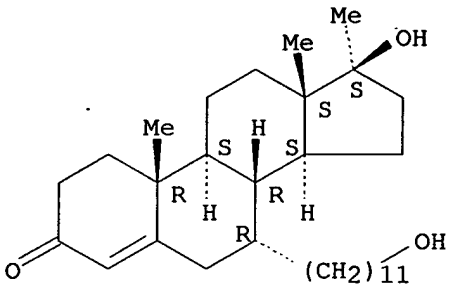
RN 278604-38-9 HCAPLUS
CN Androst-4-en-3-one, 17-(acetyloxy)-7-(11-hydroxyundecyl)-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



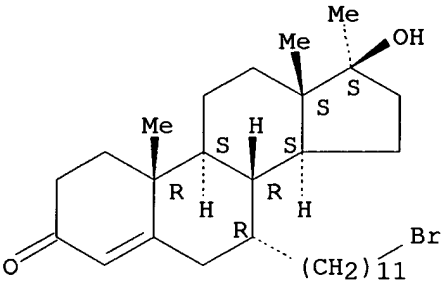
RN 278604-39-0 HCAPLUS
CN Androst-4-en-3-one, 17-hydroxy-7-(11-hydroxyundecyl)-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 278604-40-3 HCAPLUS
CN Androst-4-en-3-one, 7-(11-bromoundecyl)-17-hydroxy-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 278604-41-4 HCAPLUS
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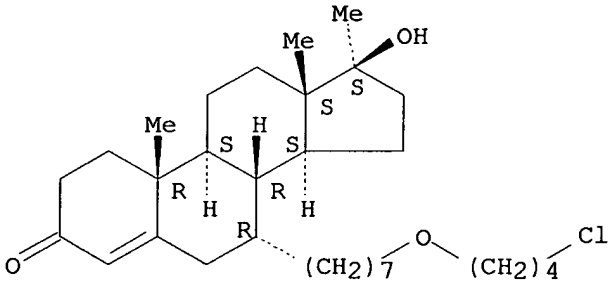
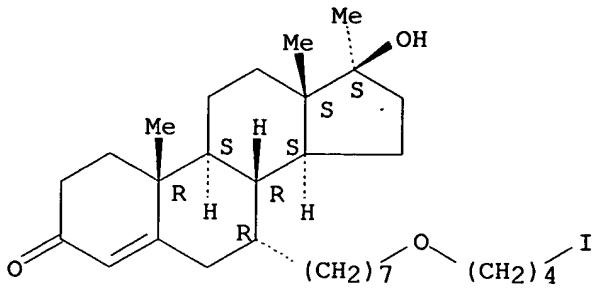
Absolute stereochemistry.



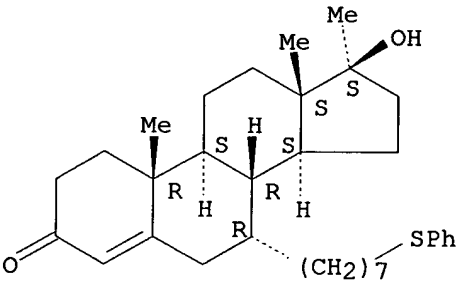
RN 278604-42-5 HCAPLUS
CN Androst-4-en-3-one, 17-hydroxy-7-[7-(4-iodobutoxy)heptyl]-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



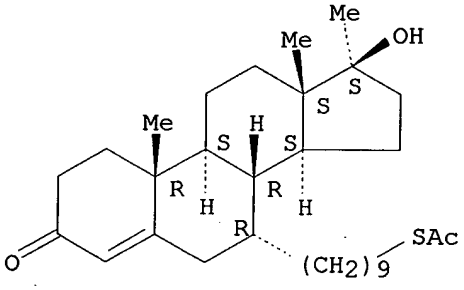
RN 278604-43-6 HCAPLUS
CN Androst-4-en-3-one, 17-hydroxy-17-methyl-7-[7-(phenylthio)heptyl]-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



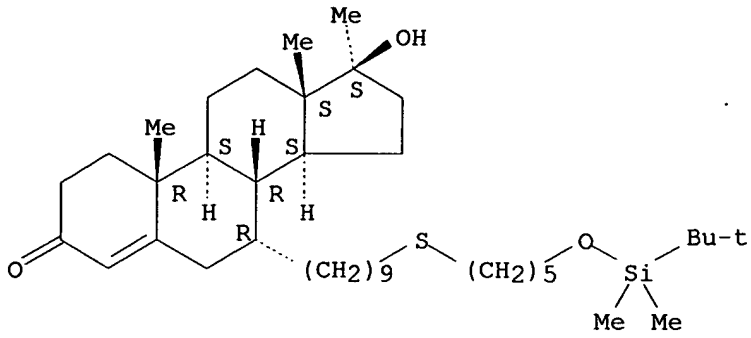
RN 278604-46-9 HCAPLUS
CN Androst-4-en-3-one, 7-[9-(acetylthio)nonyl]-17-hydroxy-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



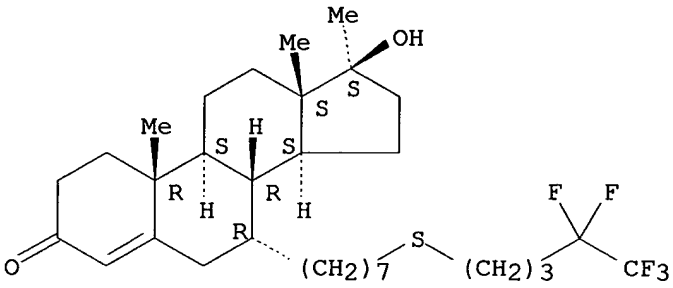
RN 278604-52-7 HCAPLUS
CN Androst-4-en-3-one, 7-[9-[[5-[[(1,1-dimethylethyl)dimethylsilyl]oxy]pentyl]thio]nonyl]-17-hydroxy-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



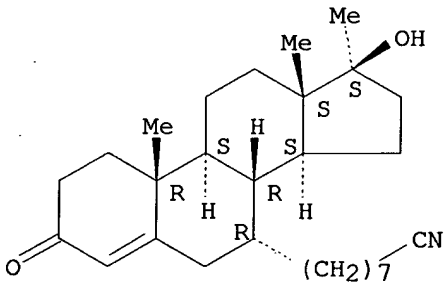
RN 278604-57-2 HCAPLUS
CN Androst-4-en-3-one, 17-hydroxy-17-methyl-7-[7-[(4,4,5,5,5-pentafluoropentyl)thio]heptyl]-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



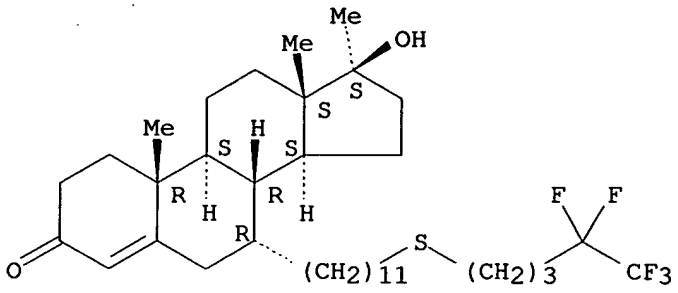
RN 278604-60-7 HCAPLUS
CN Androst-4-ene-7-octanenitrile, 17-hydroxy-17-methyl-3-oxo-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



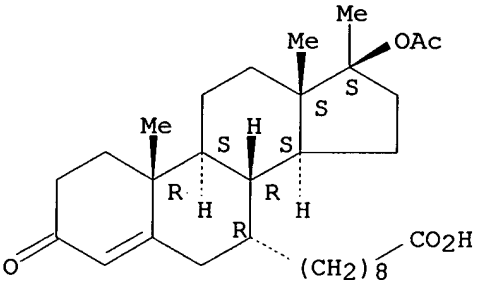
RN 278604-66-3 HCAPLUS
CN Androst-4-en-3-one, 17-hydroxy-17-methyl-7-[11-[(4,4,5,5,5-pentafluoropentyl)thio]undecyl]-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



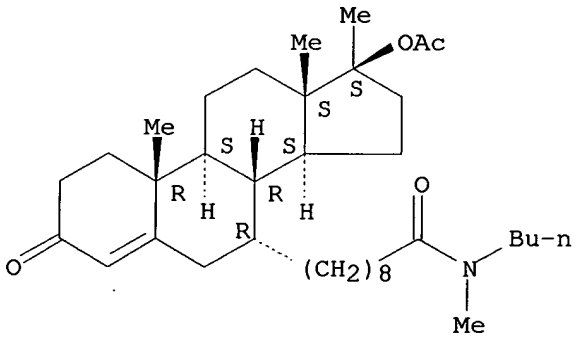
RN 278604-79-8 HCAPLUS
CN Androst-4-ene-7-nonanoic acid, 17-(acetyloxy)-17-methyl-3-oxo-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



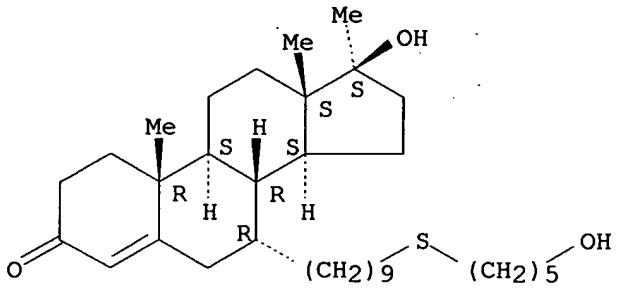
RN 278604-80-1 HCAPLUS
CN Androst-4-ene-7-nonanamide, 17-(acetyloxy)-N-butyl-N,17-dimethyl-3-oxo-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



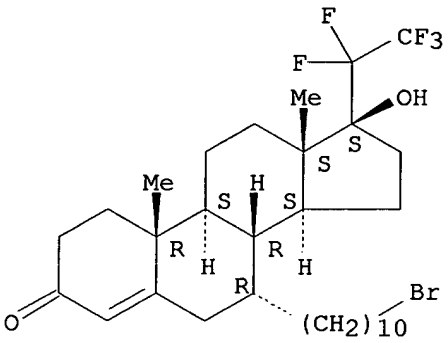
RN 278605-00-8 HCAPLUS
CN Androst-4-en-3-one, 17-hydroxy-7-[9-[(5-hydroxypentyl)thio]nonyl]-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



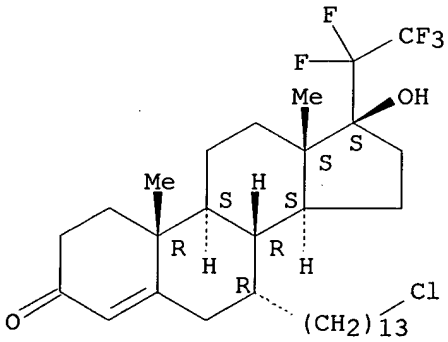
RN 278605-02-0 HCAPLUS
CN Pregn-4-en-3-one, 7-(10-bromodecyl)-20,20,21,21,21-pentafluoro-17-hydroxy-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



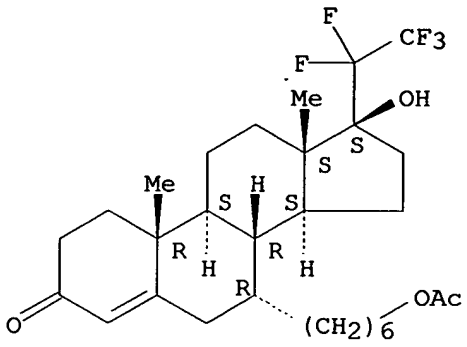
RN 278605-05-3 HCAPLUS
CN Pregn-4-en-3-one, 7-(13-chlorotridecyl)-20,20,21,21,21-pentafluoro-17-hydroxy-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 278605-09-7 HCAPLUS
CN Pregn-4-en-3-one, 7-[6-(acetyloxy)hexyl]-20,20,21,21,21-pentafluoro-17-hydroxy-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT **278603-70-6P 278603-74-0P 278603-75-1P**
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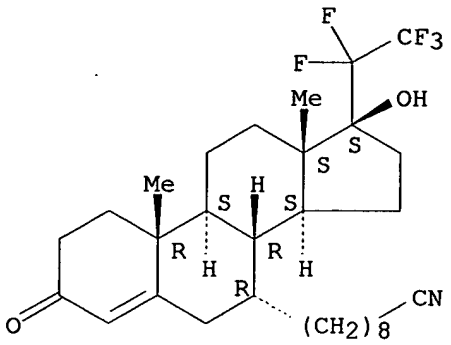
278604-91-4P 278604-92-5P 278604-93-6P
278604-94-7P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of new testosterone derivs. and their use in the long-term therapy of androgen-dependent illnesses)

RN 278603-70-6 HCAPLUS

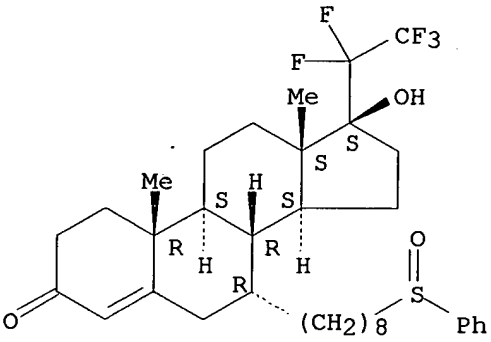
CN Pregn-4-ene-7-nonanenitrile, 20,20,21,21,21-pentafluoro-17-hydroxy-3-oxo-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



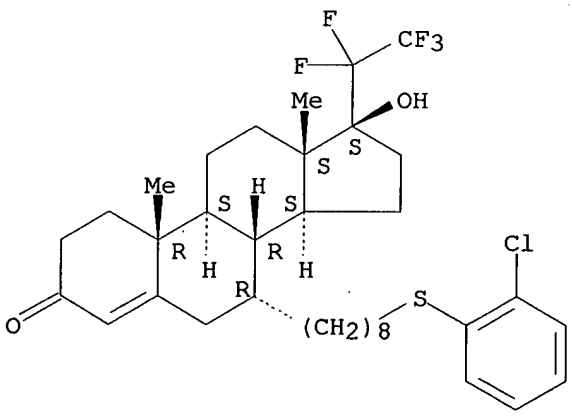
RN 278603-74-0 HCAPLUS
CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[8-(phenylsulfinyl)octyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 278603-75-1 HCAPLUS
CN Pregn-4-en-3-one, 7-[8-[(2-chlorophenyl)thio]octyl]-20,20,21,21,21-pentafluoro-17-hydroxy-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

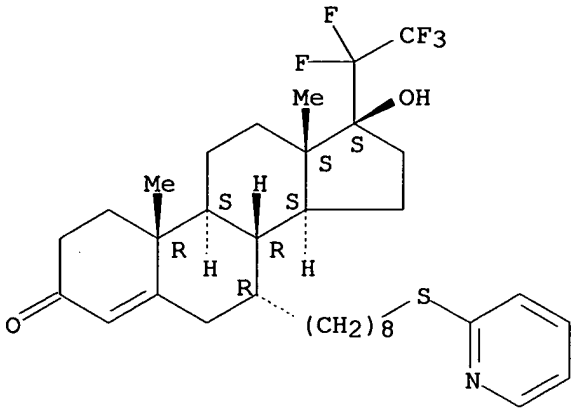
Absolute stereochemistry.



RN 278603-76-2 HCAPLUS

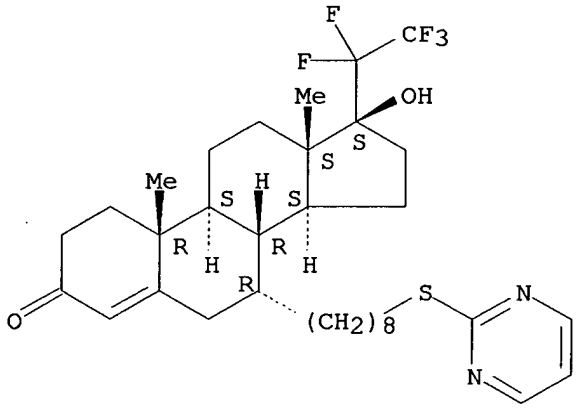
CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[8-(2-pyridinylthio)octyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



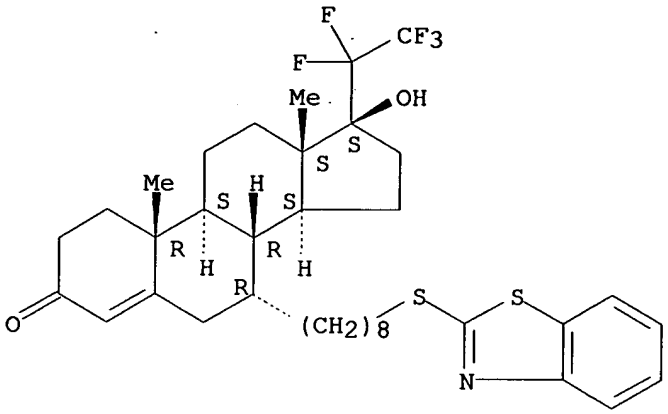
RN 278603-77-3 HCAPLUS
CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[8-(2-pyrimidinylthio)octyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



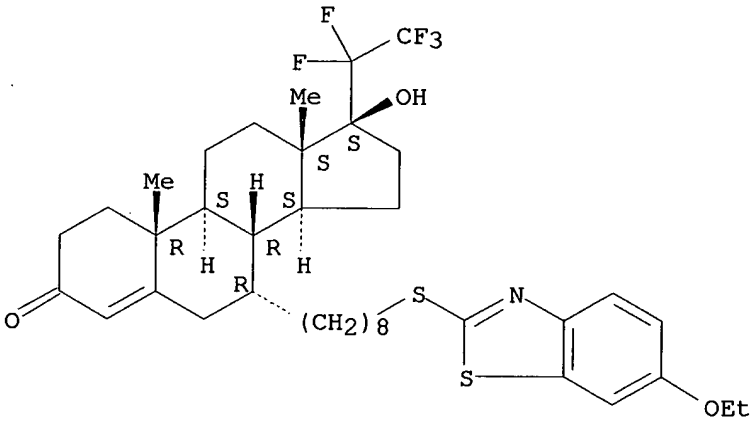
RN 278603-79-5 HCAPLUS
CN Pregn-4-en-3-one, 7-[8-(2-benzothiazolylthio)octyl]-20,20,21,21,21-pentafluoro-17-hydroxy-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



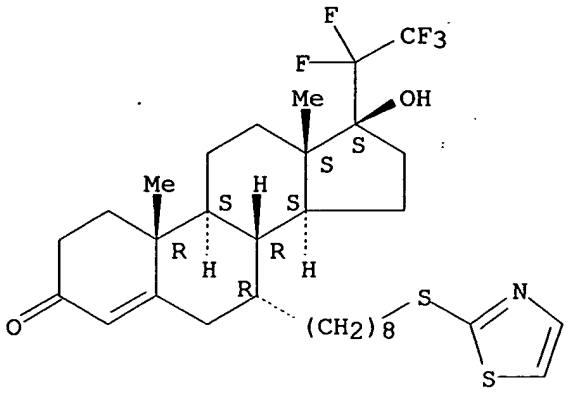
RN 278603-81-9 HCAPLUS
CN Pregn-4-en-3-one, 7-[8-[(6-ethoxy-2-benzothiazolyl)thio]octyl]-20,20,21,21,21-pentafluoro-17-hydroxy-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



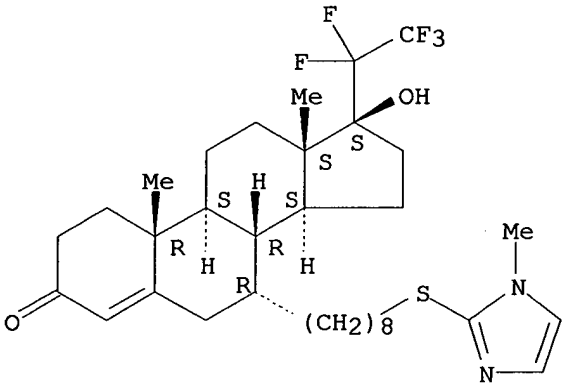
RN 278603-82-0 HCAPLUS
CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[8-(2-thiazolylthio)octyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



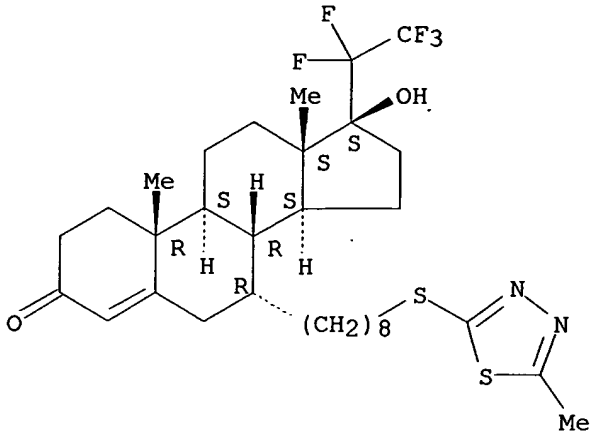
RN 278603-83-1 HCAPLUS
CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[8-[(1-methyl-1H-imidazol-2-yl)thio]octyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



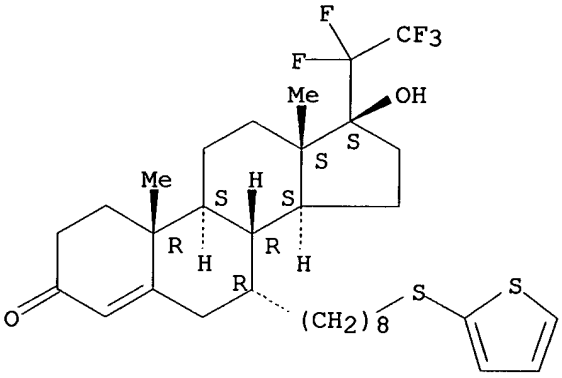
RN 278603-84-2 HCAPLUS
CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[8-[(5-methyl-1,3,4-thiadiazol-2-yl)thio]octyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



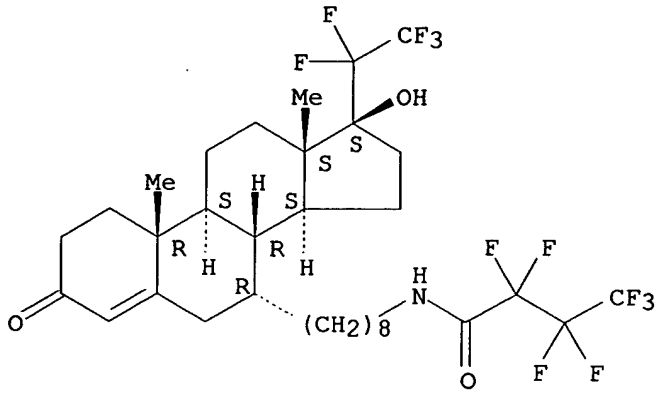
RN 278603-85-3 HCAPLUS
CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[8-(2-thienylthio)octyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



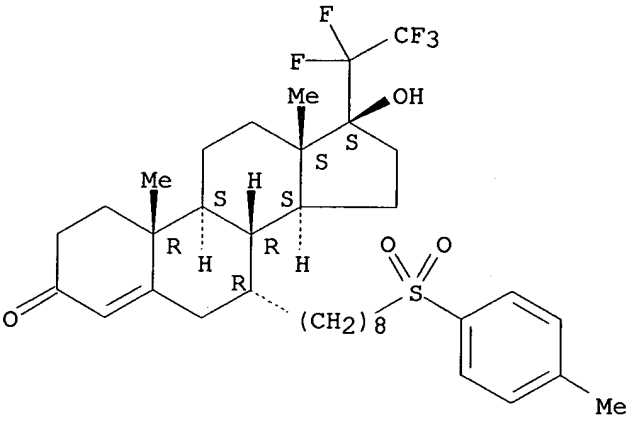
RN 278603-86-4 HCAPLUS
CN Butanamide, 2,2,3,3,4,4,4-heptafluoro-N-[8-[(7.alpha.,17.alpha.)-20,20,21,21,21-pentafluoro-17-hydroxy-3-oxopregn-4-en-7-yl]octyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



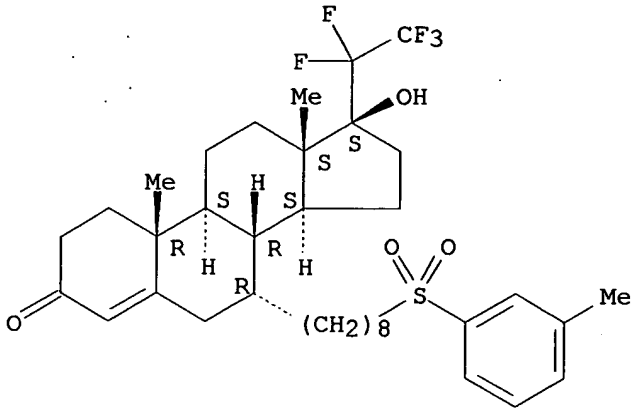
RN 278603-88-6 HCAPLUS
CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[8-[(4-methylphenyl)sulfonyl]octyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



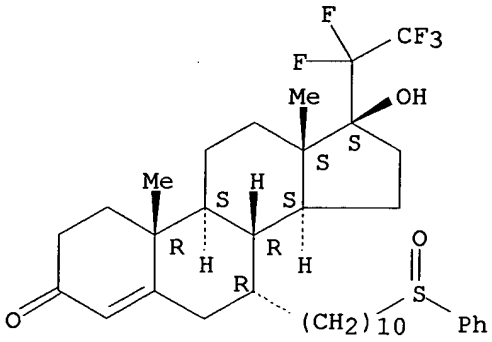
RN 278603-89-7 HCAPLUS
CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[8-[(3-methylphenyl)sulfonyl]octyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



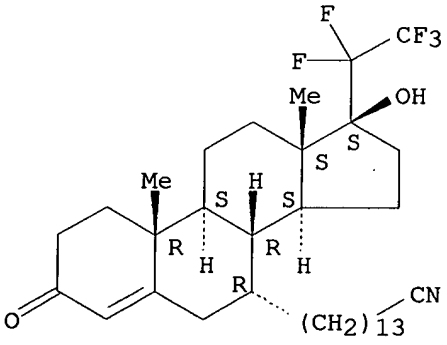
RN 278603-94-4 HCAPLUS
CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[10-(phenylsulfinyl)decyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 278603-98-8 HCAPLUS
CN Pregn-4-ene-7-tetradecanenitrile, 20,20,21,21,21-pentafluoro-17-hydroxy-3-oxo-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

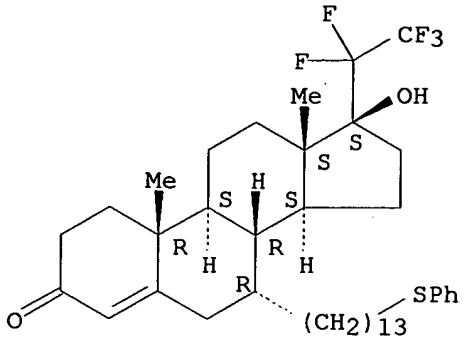
Absolute stereochemistry.



RN 278604-00-5 HCAPLUS

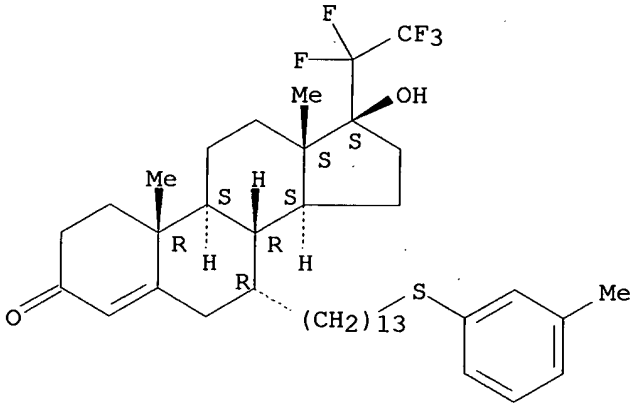
CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[13-(phenylthio)tridecyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



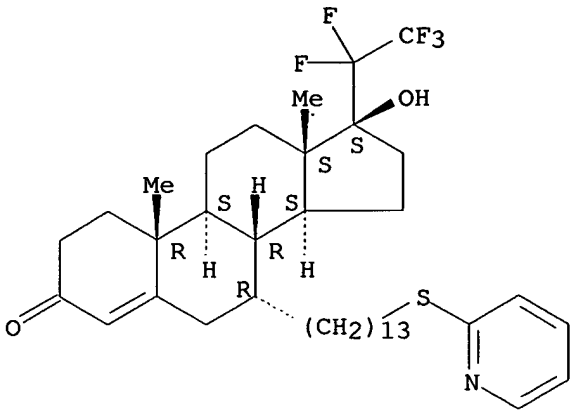
RN 278604-01-6 HCAPLUS
CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[13-[(3-methylphenyl)thio]tridecyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



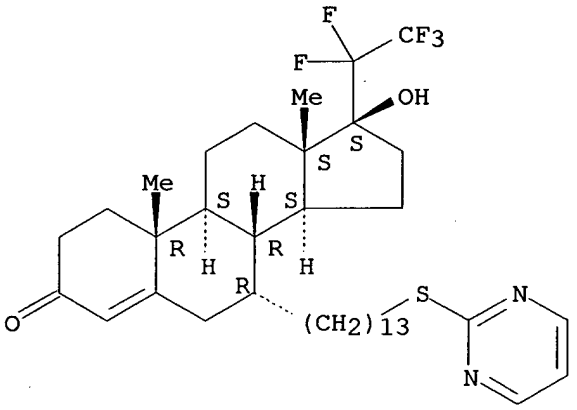
RN 278604-02-7 HCAPLUS
CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[13-(2-pyridinylthio)tridecyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



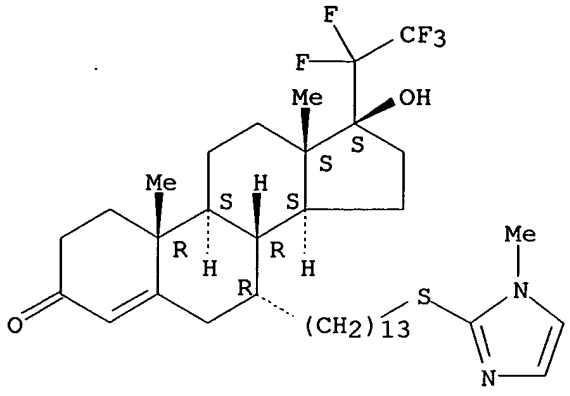
RN 278604-03-8 HCAPLUS
CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[13-(2-pyrimidinylthio)tridecyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



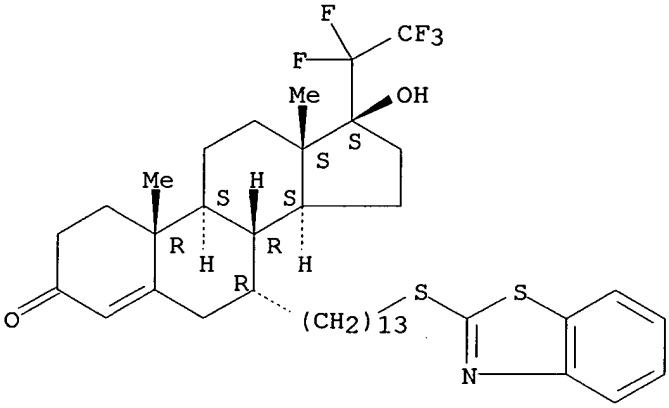
RN 278604-04-9 HCAPLUS
CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[13-[(1-methyl-1H-imidazol-2-yl)thio]tridecyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



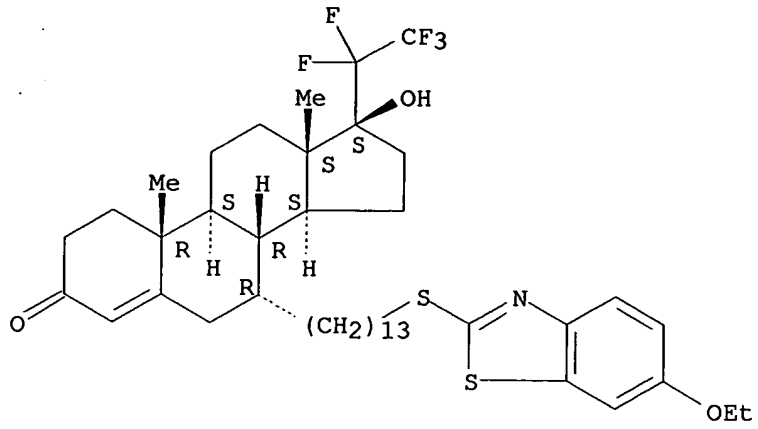
RN 278604-05-0 HCAPLUS
CN Pregn-4-en-3-one, 7-[13-(2-benzothiazolylthio)tridecyl]-20,20,21,21,21-pentafluoro-17-hydroxy-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



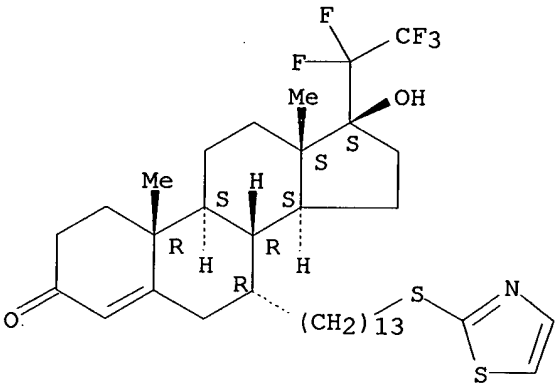
RN 278604-06-1 HCAPLUS
CN Pregn-4-en-3-one, 7-[13-[(6-ethoxy-2-benzothiazolyl)thio]tridecyl]-20,20,21,21,21-pentafluoro-17-hydroxy-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



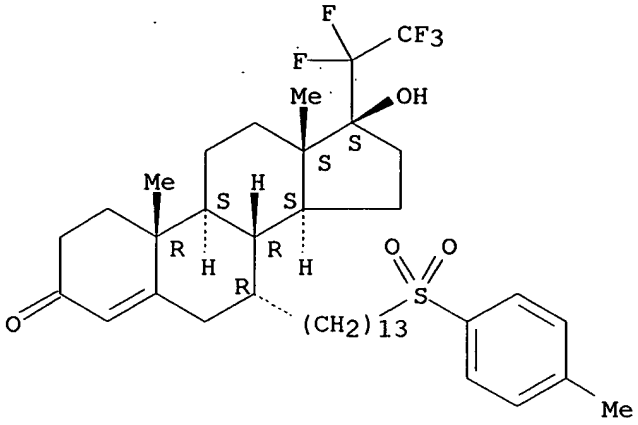
RN 278604-07-2 HCAPLUS
CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[13-(2-thiazolylthio)tridecyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



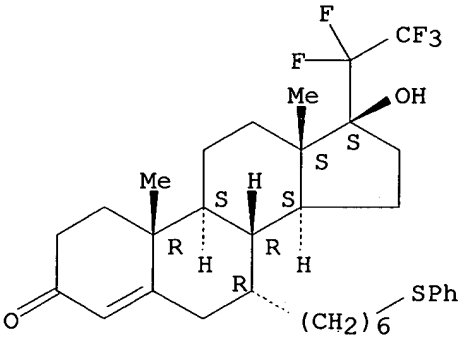
RN 278604-08-3 HCAPLUS
CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[13-[(4-methylphenyl)sulfonyl]tridecyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



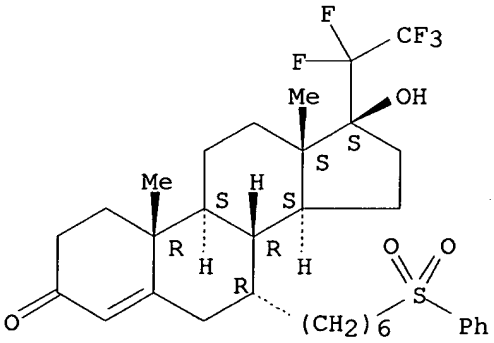
RN 278604-13-0 HCAPLUS
CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[6-(phenylthio)hexyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



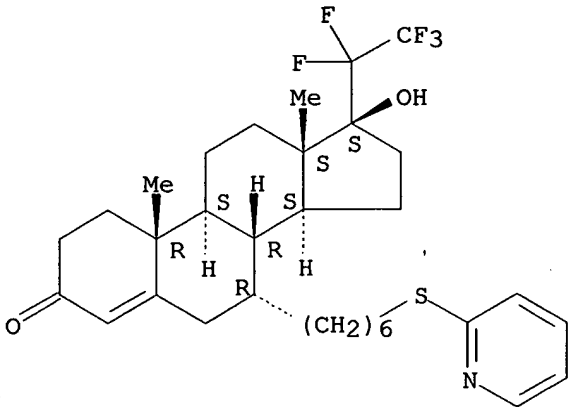
RN 278604-14-1 HCAPLUS
CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[6-(phenylsulfonyl)hexyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



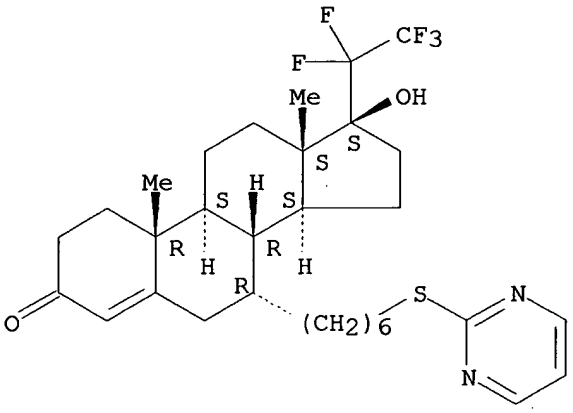
RN 278604-15-2 HCAPLUS
CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[6-(2-pyridinylthio)hexyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



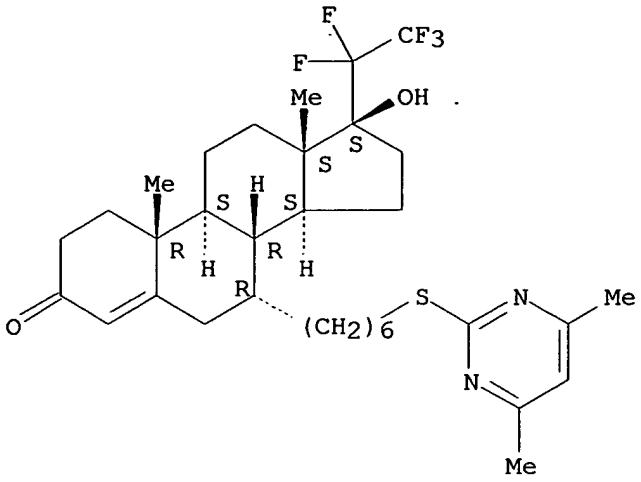
RN 278604-16-3 HCAPLUS
CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[6-(2-pyrimidinylthio)hexyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



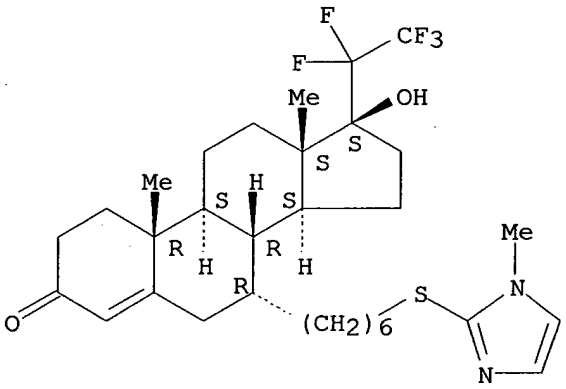
RN 278604-17-4 HCAPLUS
CN Pregn-4-en-3-one, 7-[6-[(4,6-dimethyl-2-pyrimidinyl)thio]hexyl]-20,20,21,21,21-pentafluoro-17-hydroxy-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



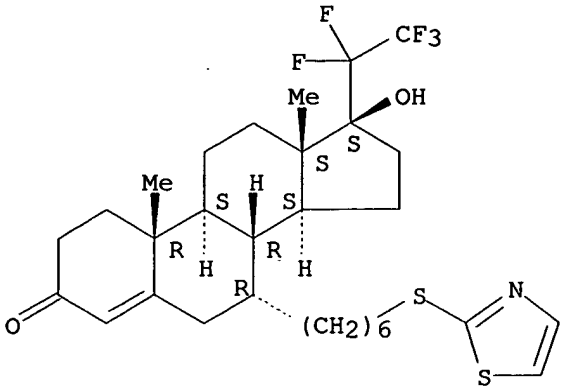
RN 278604-18-5 HCAPLUS
CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[6-[(1-methyl-1H-imidazol-2-yl)thio]hexyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



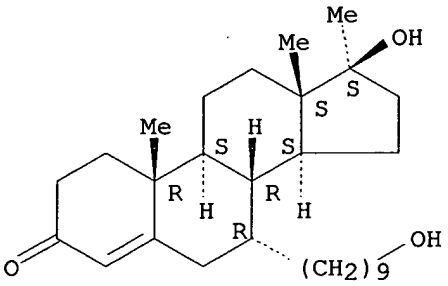
RN 278604-19-6 HCAPLUS
CN Pregn-4-en-3-one, 20,20,21,21,21-pentafluoro-17-hydroxy-7-[6-(2-thiazolylthio)hexyl]-, (7.alpha.,17.alpha.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



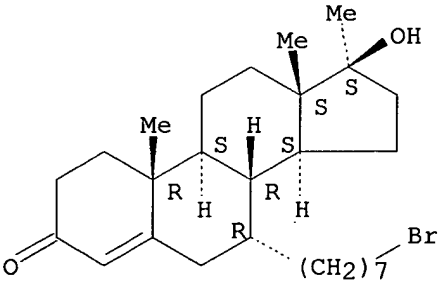
RN 278604-29-8 HCAPLUS
CN Androst-4-en-3-one, 17-hydroxy-7-(9-hydroxynonyl)-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



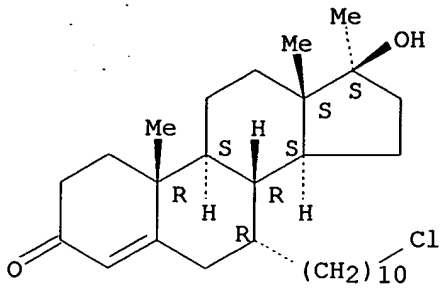
RN 278604-34-5 HCAPLUS
CN Androst-4-en-3-one, 7-(7-bromoheptyl)-17-hydroxy-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



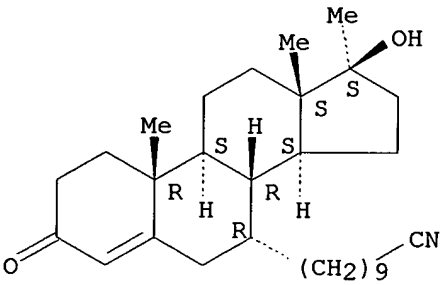
RN 278604-37-8 HCAPLUS
CN Androst-4-en-3-one, 7-(10-chlorodecyl)-17-hydroxy-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



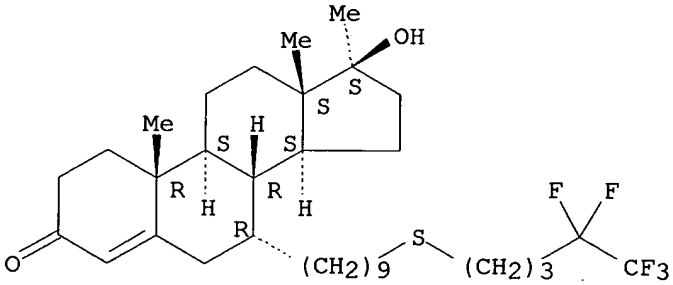
RN 278604-44-7 HCAPLUS
CN Androst-4-ene-7-decanenitrile, 17-hydroxy-17-methyl-3-oxo-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



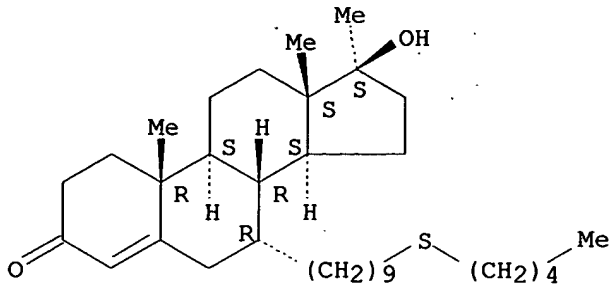
RN 278604-45-8 HCAPLUS
CN Androst-4-en-3-one, 17-hydroxy-17-methyl-7-[9-[(4,4,5,5,5-pentafluoropentyl)thio]nonyl]-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



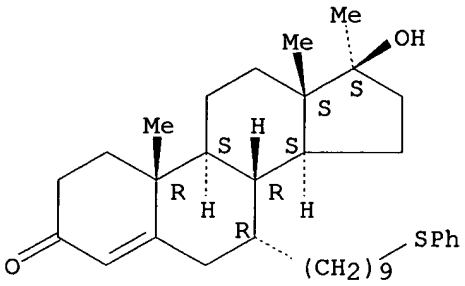
RN 278604-47-0 HCAPLUS
CN Androst-4-en-3-one, 17-hydroxy-17-methyl-7-[9-(pentylthio)nonyl]-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



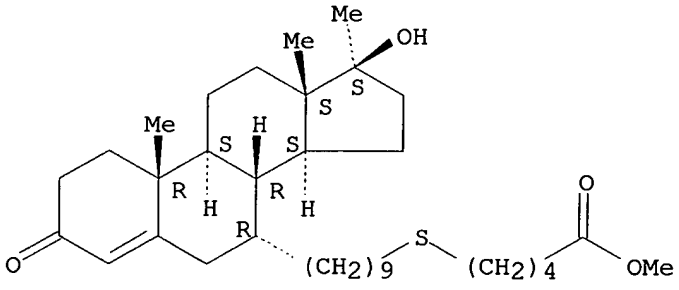
RN 278604-48-1 HCAPLUS
CN Androst-4-en-3-one, 17-hydroxy-17-methyl-7-[9-(phenylthio)nonyl]-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



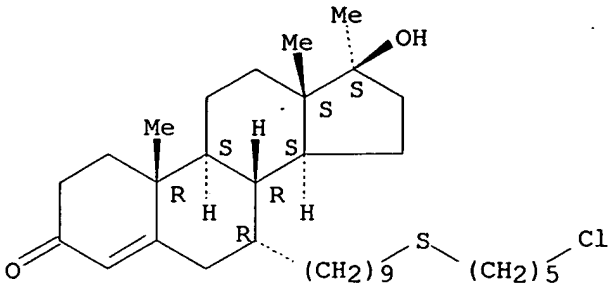
RN 278604-49-2 HCAPLUS
CN Pentanoic acid, 5-[[9-[(7.alpha.,17.beta.)-17-hydroxy-17-methyl-3-oxoandrost-4-en-7-yl]nonyl]thio]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



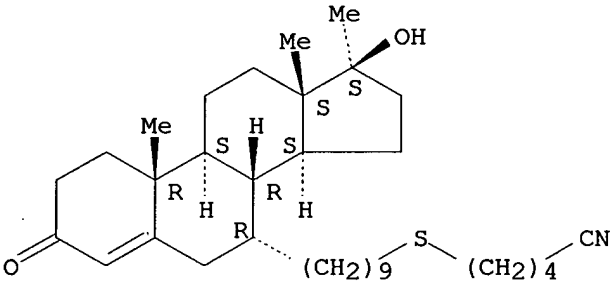
RN 278604-50-5 HCAPLUS
CN Androst-4-en-3-one, 7-[9-[(5-chloropentyl)thio]nonyl]-17-hydroxy-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



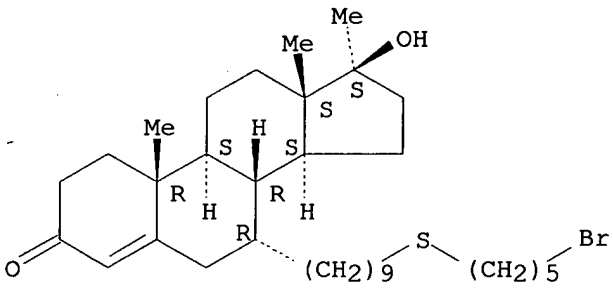
RN 278604-51-6 HCAPLUS
CN Pentanenitrile, 5-[[9-[(7.alpha.,17.beta.)-17-hydroxy-17-methyl-3-oxoandrost-4-en-7-yl]nonyl]thio]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



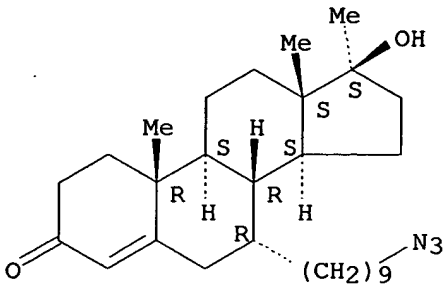
RN 278604-53-8 HCAPLUS
CN Androst-4-en-3-one, 7-[9-[(5-bromopentyl)thio]nonyl]-17-hydroxy-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



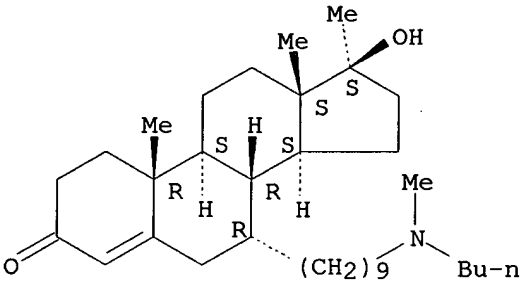
RN 278604-54-9 HCAPLUS
CN Androst-4-en-3-one, 7-(9-azidononyl)-17-hydroxy-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



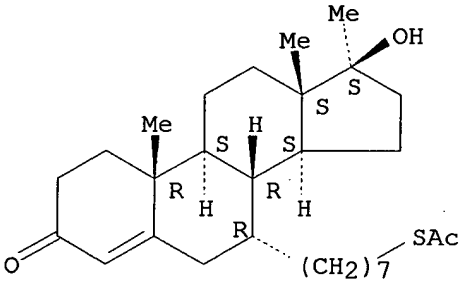
RN 278604-55-0 HCAPLUS
CN Androst-4-en-3-one, 7-[9-(butylmethylamino)nonyl]-17-hydroxy-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



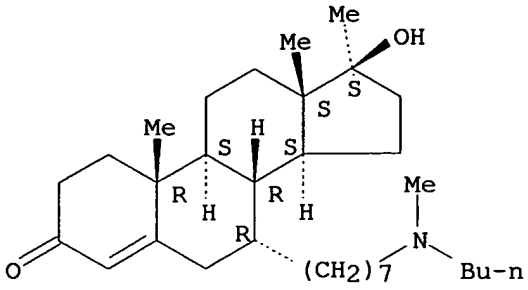
RN 278604-56-1 HCAPLUS
CN Androst-4-en-3-one, 7-[7-(acetylthio)heptyl]-17-hydroxy-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



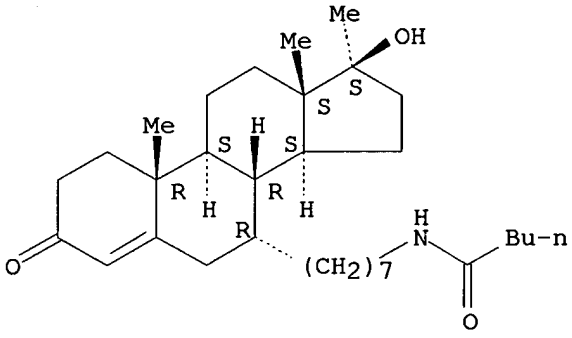
RN 278604-58-3 HCAPLUS
CN Androst-4-en-3-one, 7-[7-(butylmethylamino)heptyl]-17-hydroxy-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



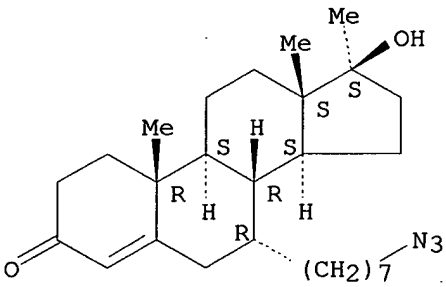
RN 278604-59-4 HCAPLUS
CN Pentanamide, N-[7-[(7.alpha.,17.beta.)-17-hydroxy-17-methyl-3-oxoandrost-4-en-7-yl]heptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



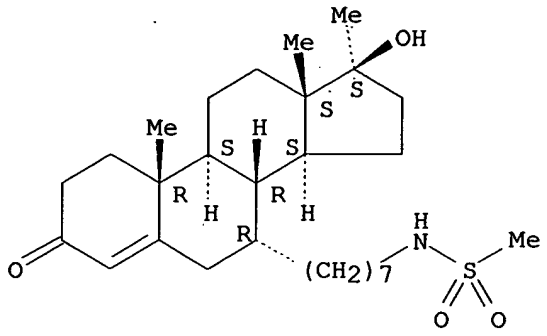
RN 278604-61-8 HCAPLUS
CN Androst-4-en-3-one, 7-(7-azidoheptyl)-17-hydroxy-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



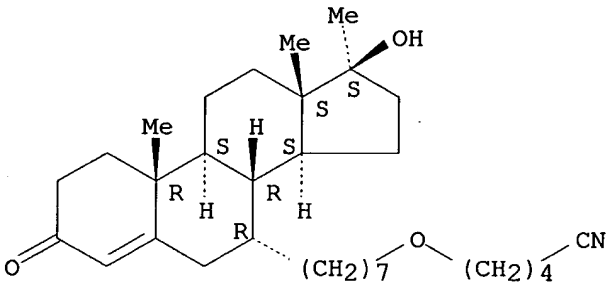
RN 278604-62-9 HCAPLUS
CN Methanesulfonamide, N-[7-[(7.alpha.,17.beta.)-17-hydroxy-17-methyl-3-oxoandrost-4-en-7-yl]heptyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



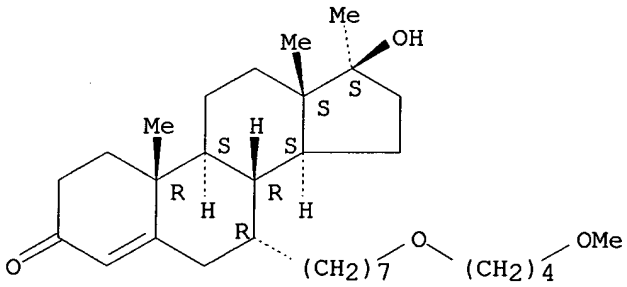
RN 278604-63-0 HCAPLUS
CN Pentanenitrile, 5-[[7-[(7.alpha.,17.beta.)-17-hydroxy-17-methyl-3-oxoandrost-4-en-7-yl]heptyl]oxy]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



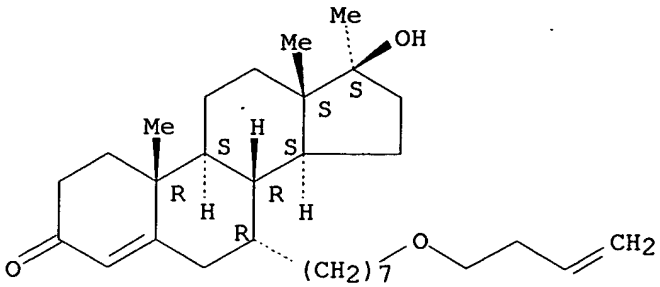
RN 278604-64-1 HCAPLUS
CN Androst-4-en-3-one, 17-hydroxy-7-[7-(4-methoxybutoxy)heptyl]-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



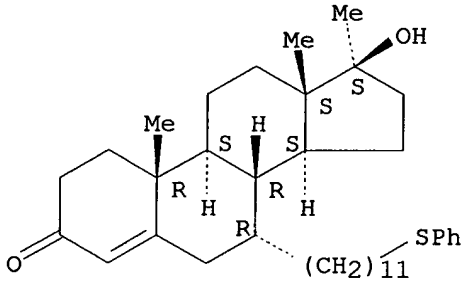
RN 278604-65-2 HCAPLUS
CN Androst-4-en-3-one, 7-[7-(3-butenyloxy)heptyl]-17-hydroxy-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



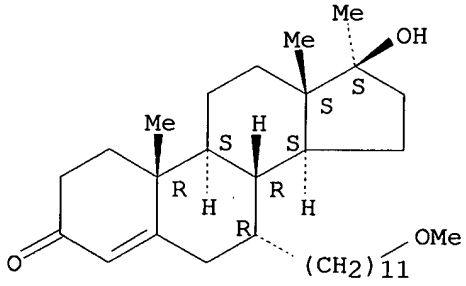
RN 278604-67-4 HCAPLUS
CN Androst-4-en-3-one, 17-hydroxy-17-methyl-7-[11-(phenylthio)undecyl]-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



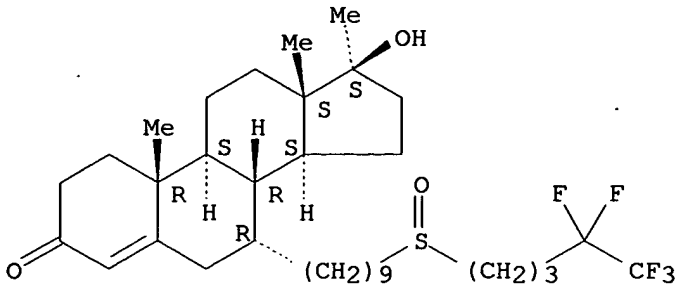
RN 278604-68-5 HCAPLUS
CN Androst-4-en-3-one, 17-hydroxy-7-(11-methoxyundecyl)-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



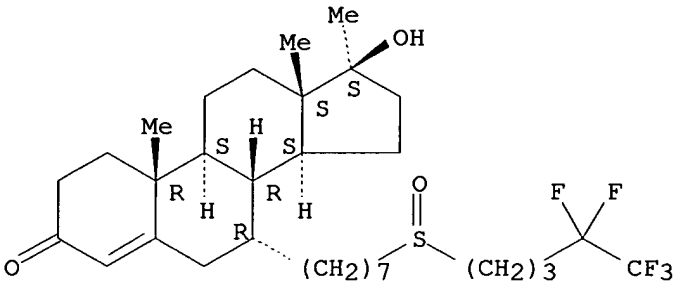
RN 278604-69-6 HCAPLUS
CN Androst-4-en-3-one, 17-hydroxy-17-methyl-7-[9-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]nonyl]-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



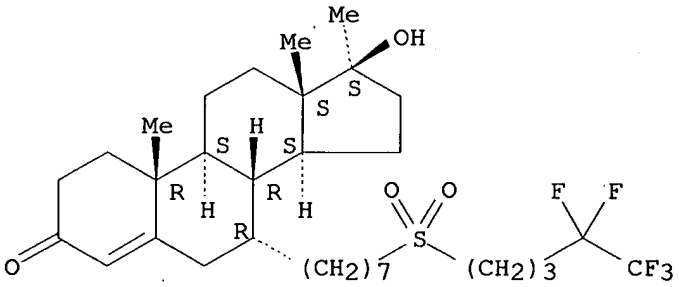
RN 278604-70-9 HCAPLUS
CN Androst-4-en-3-one, 17-hydroxy-17-methyl-7-[7-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]heptyl]-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



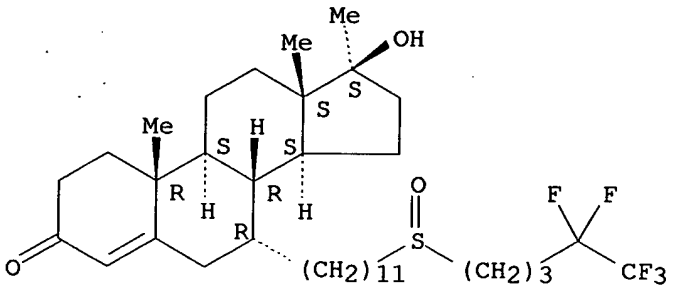
RN 278604-71-0 HCAPLUS
CN Androst-4-en-3-one, 17-hydroxy-17-methyl-7-[7-[(4,4,5,5,5-pentafluoropentyl)sulfonyl]heptyl]-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



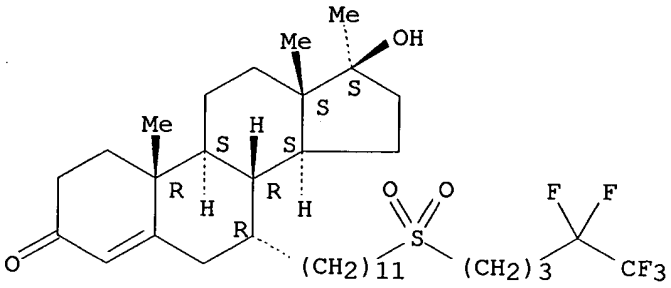
RN 278604-72-1 HCAPLUS
CN Androst-4-en-3-one, 17-hydroxy-17-methyl-7-[11-[(4,4,5,5,5-pentafluoropentyl)sulfinyl]undecyl]-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



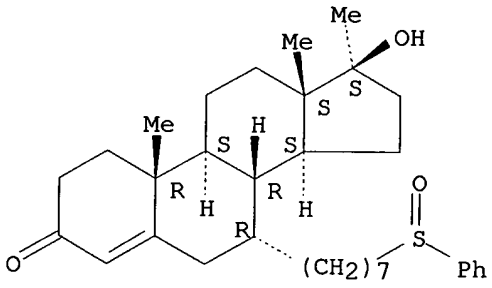
RN 278604-73-2 HCAPLUS
CN Androst-4-en-3-one, 17-hydroxy-17-methyl-7-[11-[(4,4,5,5,5-pentafluoropentyl)sulfonyl]undecyl]-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



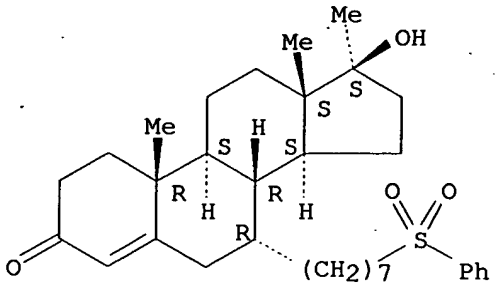
RN 278604-74-3 HCAPLUS
CN Androst-4-en-3-one, 17-hydroxy-17-methyl-7-[7-(phenylsulfinyl)heptyl]-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



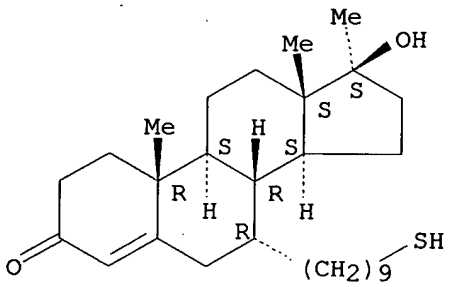
RN 278604-75-4 HCAPLUS
CN Androst-4-en-3-one, 17-hydroxy-17-methyl-7-[7-(phenylsulfonyl)heptyl]-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



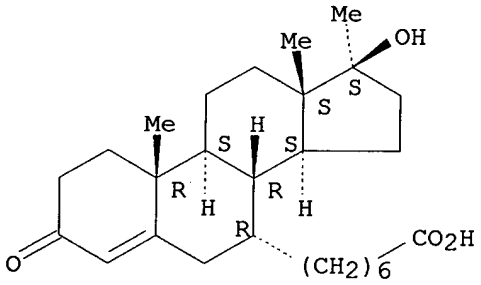
RN 278604-76-5 HCAPLUS
CN Androst-4-en-3-one, 17-hydroxy-7-(9-mercaptononyl)-17-methyl-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



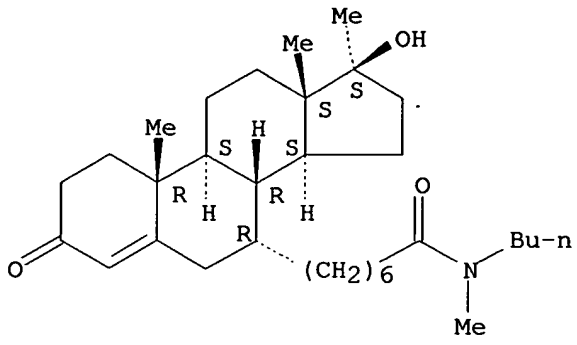
RN 278604-77-6 HCAPLUS
CN Androst-4-ene-7-heptanoic acid, 17-hydroxy-17-methyl-3-oxo-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



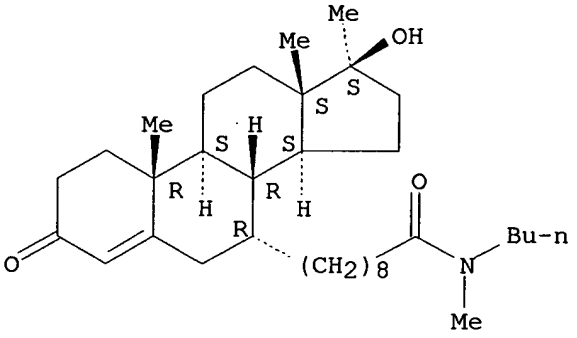
RN 278604-78-7 HCAPLUS
CN Androst-4-ene-7-heptanamide, N-butyl-17-hydroxy-N,17-dimethyl-3-oxo-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



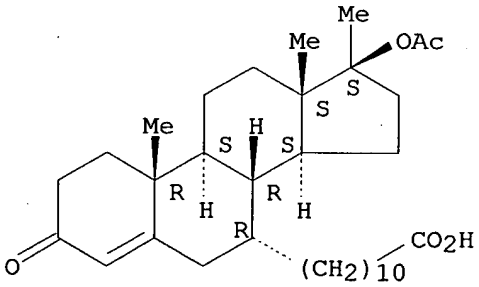
RN 278604-81-2 HCAPLUS
CN Androst-4-ene-7-nonanamide, N-butyl-17-hydroxy-N,17-dimethyl-3-oxo-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



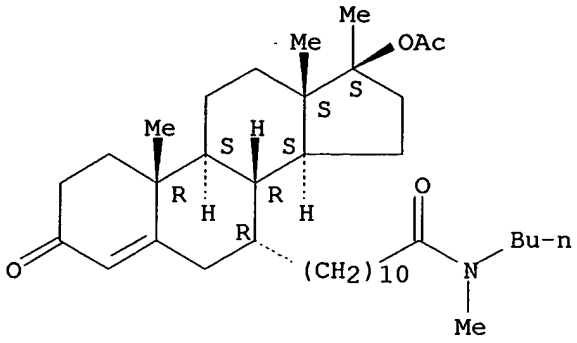
RN 278604-82-3 HCAPLUS
CN Androst-4-ene-7-undecanoic acid, 17-(acetyloxy)-17-methyl-3-oxo-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



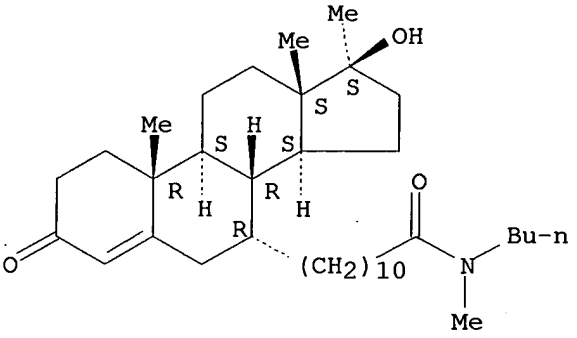
RN 278604-83-4 HCAPLUS
CN Androst-4-ene-7-undecanamide, 17-(acetyloxy)-N-butyl-N,17-dimethyl-3-oxo-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



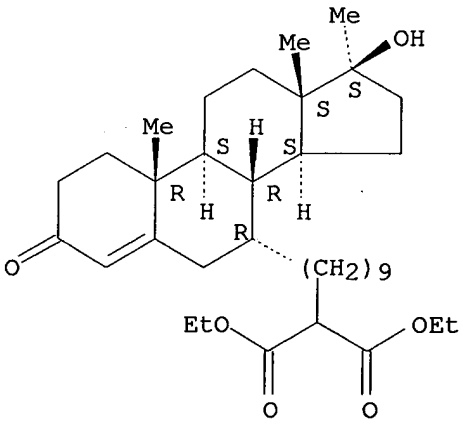
RN 278604-84-5 HCAPLUS
CN Androst-4-ene-7-undecanamide, N-butyl-17-hydroxy-N,17-dimethyl-3-oxo-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



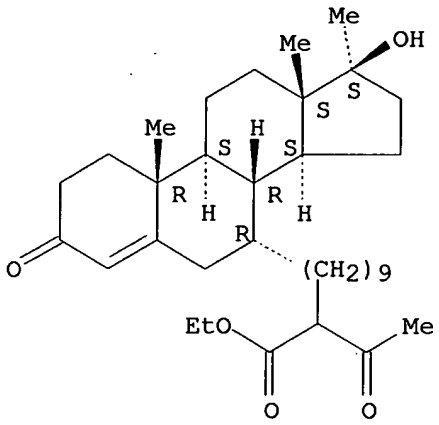
RN 278604-85-6 HCAPLUS
CN Propanedioic acid, [9-[(7.alpha.,17.beta.)-17-hydroxy-17-methyl-3-oxoandrost-4-en-7-yl]nonyl]-, diethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



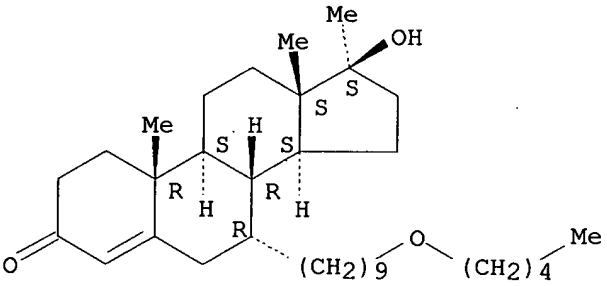
RN 278604-86-7 HCAPLUS
CN Androst-4-ene-7-undecanoic acid, .alpha.-acetyl-17-hydroxy-17-methyl-3-oxo-, ethyl ester, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



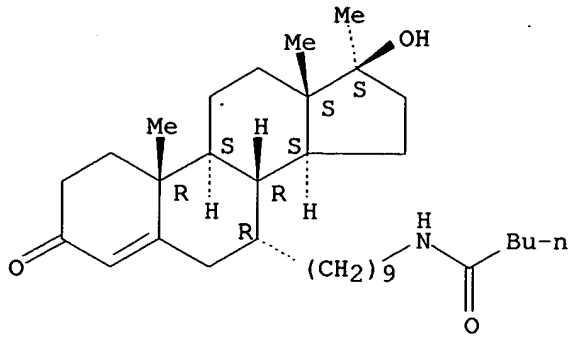
RN 278604-87-8 HCAPLUS
CN Androst-4-en-3-one, 17-hydroxy-17-methyl-7-[9-(pentyloxy)nonyl]-, (7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



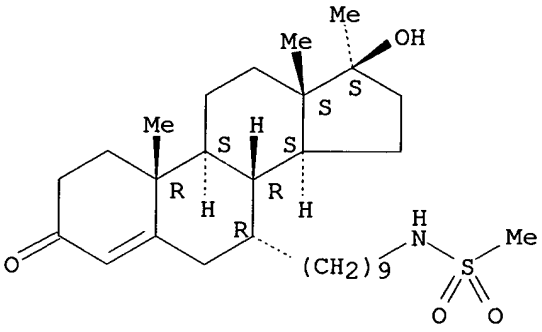
RN 278604-88-9 HCAPLUS
CN Pentanamide, N-[9-[(7.alpha.,17.beta.)-17-hydroxy-17-methyl-3-oxoandrost-4-en-7-yl]nonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



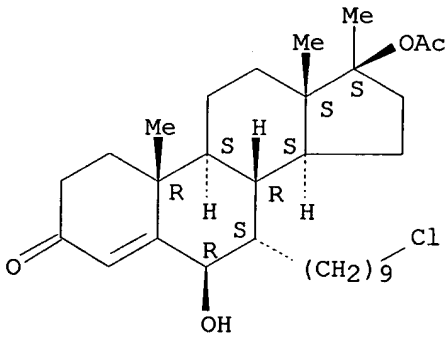
RN 278604-89-0 HCAPLUS
CN Methanesulfonamide, N-[9-[(7.alpha.,17.beta.)-17-hydroxy-17-methyl-3-oxoandrost-4-en-7-yl]nonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



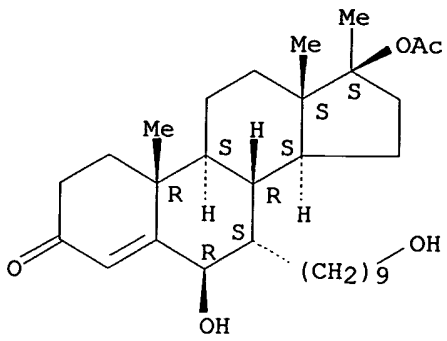
RN 278604-90-3 HCAPLUS
CN Androst-4-en-3-one, 17-(acetyloxy)-7-(9-chlorononyl)-6-hydroxy-17-methyl-, (6.beta.,7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



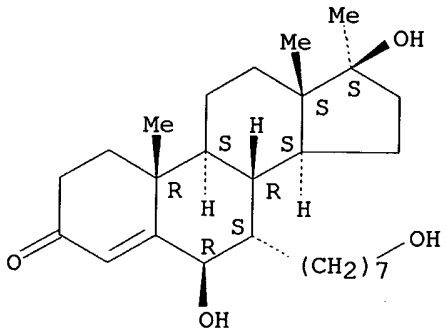
RN 278604-91-4 HCAPLUS
CN Androst-4-en-3-one, 17-(acetyloxy)-6-hydroxy-7-(9-hydroxynonyl)-17-methyl-, (6.beta.,7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



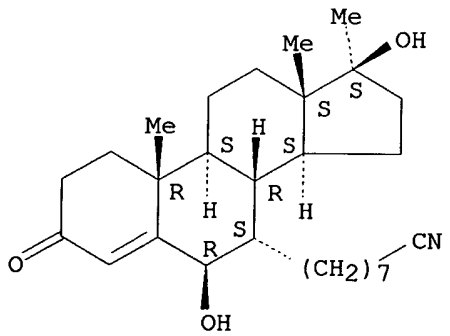
RN 278604-92-5 HCAPLUS
CN Androst-4-en-3-one, 6,17-dihydroxy-7-(7-hydroxyheptyl)-17-methyl-, (6.beta.,7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



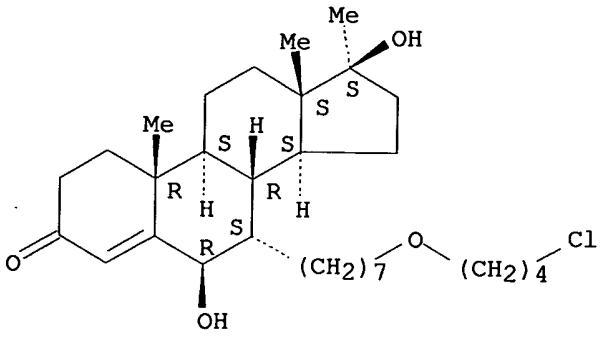
RN 278604-93-6 HCAPLUS
CN Androst-4-ene-7-octanenitrile, 6,17-dihydroxy-17-methyl-3-oxo-, (6.beta.,7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



RN 278604-94-7 HCAPLUS
CN Androst-4-en-3-one, 7-[7-(4-chlorobutoxy)heptyl]-6,17-dihydroxy-17-methyl-, (6.beta.,7.alpha.,17.beta.)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.



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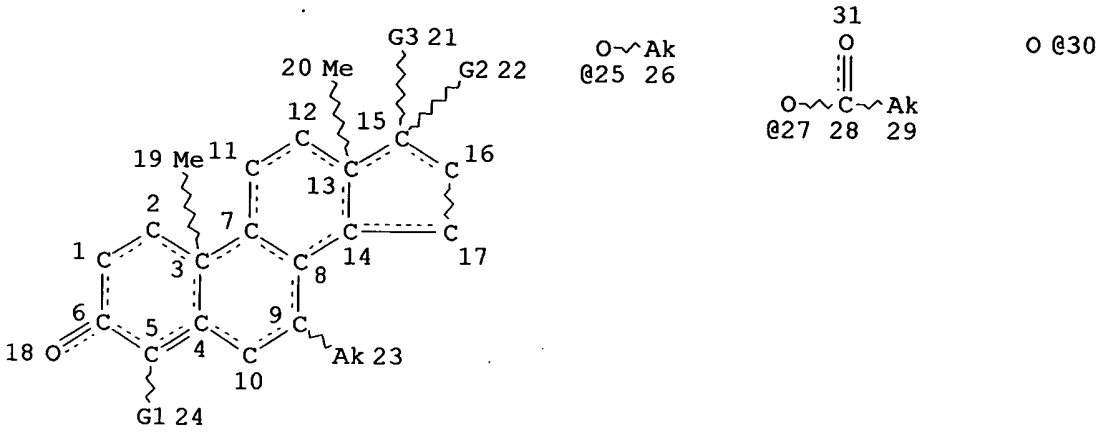
L1 STR



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GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 35

STEREO ATTRIBUTES: NONE
L6 3 SEA FILE=MARPAT SSS FUL L1
L7 1 SEA FILE=MARPAT ABB=ON PLU=ON L6/COM

=> d all

L7 ANSWER 1 OF 1 MARPAT COPYRIGHT 2003 ACS
AN 133:350394 MARPAT
TI Preparation of steroid derivatives
IN Liao, Shutsung; Song, Ching

PA Arch Development Corporation, USA
SO PCT Int. Appl., 67 pp.
CODEN: PIXXD2
DT Patent
LA English
IC ICM C07J003-00
ICS C07J009-00; C07J017-00; C07J041-00; A61K031-56; A61K031-585
CC 32-7 (Steroids)
Section cross-reference(s): 1, 63
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2000066611	A1	20001109	WO 2000-US11243	20000427
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	RW: GH, GM, KE, LS, MW, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	EP 1189922	A1	20020327	EP 2000-928431	20000427
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	BR 2000010197	A	20020716	BR 2000-10197	20000427
	JP 2002543216	T2	20021217	JP 2000-615640	20000427
	NO 2001005314	A	20011227	NO 2001-5314	20011030
PRAI	US 1999-131728P	19990430			
	US 2000-191864P	20000324			
	WO 2000-US11243	20000427			

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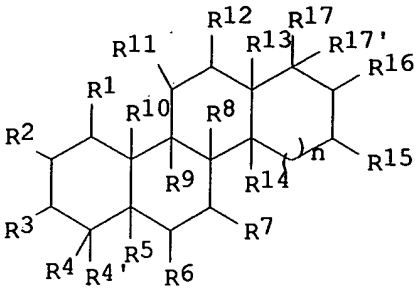

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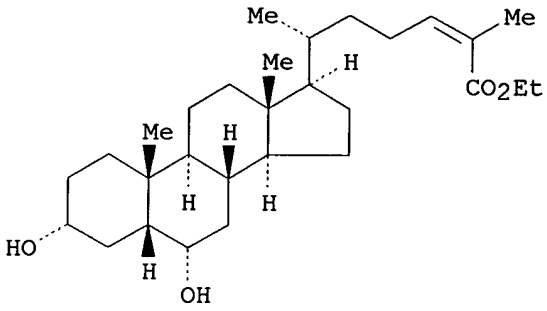


II

AB The steroid derivs. I (R3 = H, amino, carboxyl, oxo, halo, sulfonic acid, -O-sulfonic acid, or alkyl that is optionally inserted with -NH-,-N(alkyl)-, -O-, -S-, -SO-, -SO2-, -O-SO2-, -SO2-O-, -O-SO3-, -SO3-O-, -CO-, -CO-O-, -O-CO-, -CO-NH-, -CO-N(alkyl)-, -NH-CO-, or -N(alkyl)-CO-, and further optionally substituted with hydroxy, halo, amino, carboxyl, sulfonic acid, or -O-sulfonic acid),. R1, R2, R4, R4', R6, R7, R11, R12, R15, R16, and R17', independently, is H, hydroxy, amino, carboxyl, oxo, halo, sulfoic acid, -O-sulfonic acid, or alkyl that is optionally inserted with -NH-, -N(alkyl)-, -O-, -S-, -SO-, -SO2-, -O-SO2-, -SO2-0-, -O-SO3-, -SO3-O-, -CO-, -CO-O-, -O-CO-, -CO-NH-, -CO-N(alkyl)-, -NH-CO-, or -N(alkyl)-CO-, and further optionally substituted with hydroxy, halo, amino, carboxyl, sulfonic acid, or -O-sulfonic acid. R5, R8, R9, R10, R13, and R14, independently, is H, alkyl, haloalkyl, hydroxyalkyl, alkoxy, hydroxy, or amino; R17 is -X-Y-Z, in which X is a bond, or alkyl or alkenyl, optionally inserted with -NH-, -N(alkyl)-, -O-, or -S-, and further optionally forming a cyclic moiety with R16 and the 2 ring carbon atoms to which R16 and R17 are bonded; Y is -CO-, -SO-, -SO2-, -O-SO2-, -SO2-O-, -O-SO3-, -SO3-O-, -CO-O-, -O-CO-, -CO-NH-,-CO-N(alkyl)-, -NH-CO-, -N(alkyl)-CO-, or a bond. Z = alkyl, alkenyl, alkynyl, cycloalkyl, heterocycloalkyl, cycloalkenyl, heterocycloalkenyl, aryl, heteroaryl, aralkyl, or heteroaralkyl, and is optionally substituted with hydroxy, alkoxy, amino, halo, sulfonic acid, -O-sulfonic acid, carboxyl, oxo, alkyloxycarbonyl, alkylcarbonyloxy, alkylaminocarbonyl, alkylcarbonylamino, alkylcarbonyl, alkylsulfinyl, alkylsulfonyl, or alkylthio; or is -CH(A)-B with A being a side chain of an amino acid, and B being hydrogen, -NRaRb, or -COORc wherein each of Ra, Rb, and Rc, independently, is hydrogen or alkyl; n is 0, 1, or 2. Provided that when Z is substituted with carboxyl or alkyloxycarbonyl, Y is a bond and either X or Z contains at least one double bond, and that when Y is a bond,

either X is -NH-alkyl, -NH-alkenyl, -N(alkyl)-alkyl-, -N(alkyl)-alkenyl-, -O-alkyl-, -O-alkenyl-, -S-alkyl-, or -S-alkenyl-; or Z is substituted with halo, sulfonic acid, -O-sulfonic acid, alkylsulfinyl, or alkylsulfonyl, or is alkenyl or their salts were prepd. Thus, to a stirred soln. of L- (or D-) phenylalanine ester hydrochloride in dry DMF was added triethylamine and the mixt. was stirred at room temp. for 10 min, bile acid and 1-ethyl-3-[3-dimethylaminopropyl]-carbodiimide were then added and the suspension was stirred at room temp. overnight. Reaction mixt. was dild. with water and Et acetate, the org. layer was sepd. and the water layer was extd. with Et acetate again, the combined org. layer was then washed with 1N HCl, water, 1N NaOH and water, and dried (MgSO4), removed the solvent under reduced pressure to afford the steroid derivs., e.g. II. Steroid derivs. of I interact with nuclear liver X receptor (LXR) and ubiquitous receptor (UR), and can be used to treat a variety of LXR- or UR- mediated disorders.

ST steroid deriv prepn nuclear receptor

IT Nuclear receptors
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(liver X and ubiquitous; prepn. of steroid derivs.)

IT Transformation, genetic
(mammalian cell; prepn. of steroid derivs.)

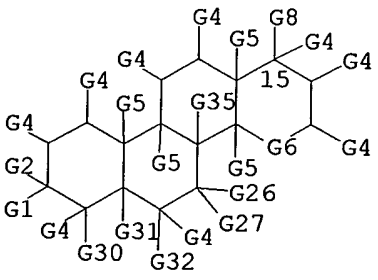
IT 1173-32-6P 1672-46-4P 2868-48-6P 10538-59-7P 115679-81-7P
300548-56-5P 300548-57-6P 305835-13-6P 305835-16-9P 305835-18-1P
305835-20-5P 305835-22-7P 305835-25-0P 305835-26-1P 305835-27-2P
305835-28-3P 305835-29-4P 305835-30-7P 305835-33-0P 305835-35-2P
305835-37-4P 305835-39-6P 305835-41-0P 305835-43-2P 305835-45-4P
305835-47-6P, Cholesta-5,24-diene-3,26-diol 305835-48-7P 305835-49-8P
305835-50-1P 305835-51-2P 305835-52-3P 305835-53-4P 305835-54-5P
306759-81-9P 306759-82-0P
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. of steroid derivs.)

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD

RE

(1) Angelico; Scandinavian Journal of Gasteroenterology 1995, V30(12), P1178 CAPLUS
(2) Ruelle; International Journal of Pharmaceutics 1997, V157(2), P219 CAPLUS
(3) Xia, P; Heterocycles 1998, V47(2), P703 CAPLUS

MSTR 1A



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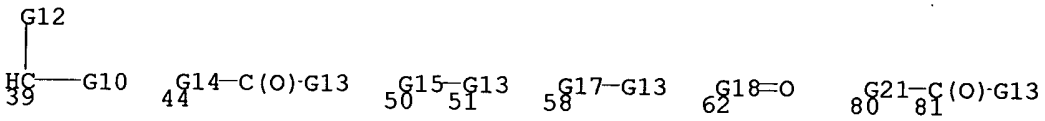
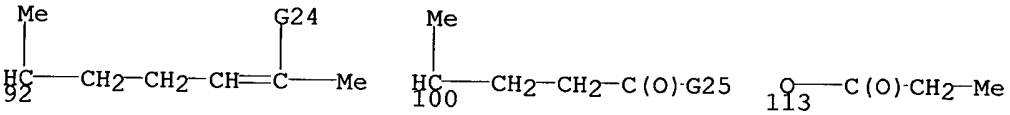
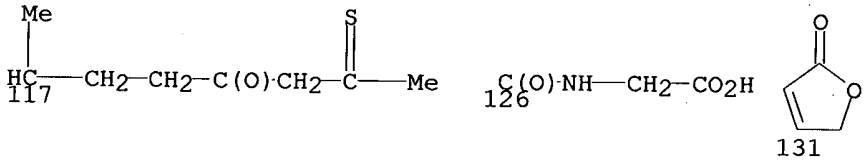
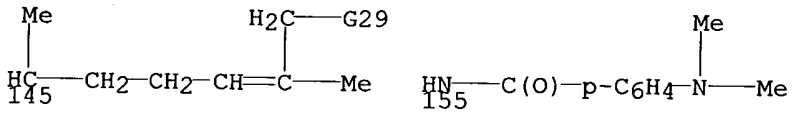
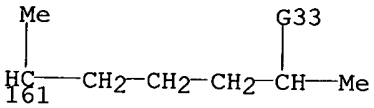
G2 = H
G3 = OH / F / Cl / Br / I / NH2 / CO2H / SO3H / OSO3H
G4 = H / OH / NH2 / CO2H / F / Cl / Br / I / SO3H / OSO3H / alkyl<(1-8)> (SO (1-) G3)
G5 = H / alkyl<(1-8)> (SO (1-) G7) / alkyl<(1-8)> (SR (1-) OH) / alkoxy<(1-8)> / OH / NH2 / (SC Me)
G6 = (0-2) CH2
G7 = F / Cl / Br / I
G8 = alkyl<(1-8)> (SO (1-) G9) / alkenyl<(2-8)> (SO) / alkynyl<(2-8)> (SO) / cycloalkyl<(3-8)> (SO) / Hy<EC (3-8) A (1-) Q, AR (0), BD (0-) D (0) T> (SO) / cycloalkenyl<(3-8)> (SO) / aryl<(6-12)> (SO) / heteroaryl<EC (-12) A (1-) Q> (SO) / 62 / 39 / 58 / 44 / 50 / 80 / (SC 92 / 100 / 113 / 117 / 126 / 131 / 145 / 155 / 161 / 169 / 183)

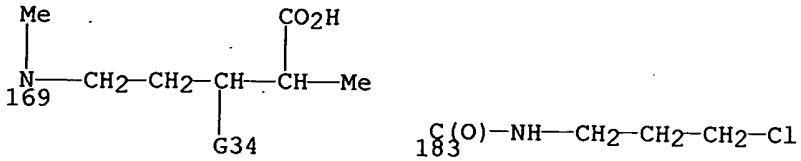




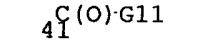




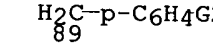




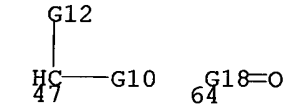
G9 = R / aryl<(6-12)> (SO) /
heteroaryl<EC (-12) A (1-) Q> (SO)
G10 = H / NH2 / alkylamino<(1-8)> / dialkylamino<(1-8)> /
41



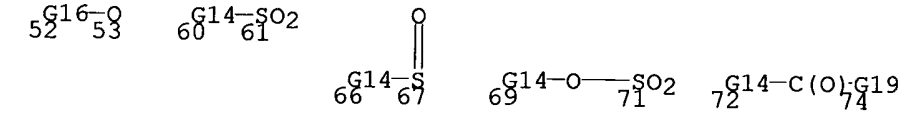
G11 = OH / alkoxy<(1-8)>
G12 = H / R<TX "side chain of amino acid"> / (SC 89)



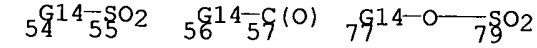
G13 = alkyl<(1-8)> (SO (1-) G9) / alkenyl<(2-8)> (SO) /
alkynyl<(2-8)> (SO) / cycloalkyl<(3-8)> (SO) /
Hy<EC (3-8) A (1-) Q, AR (0), BD (0-) D (0) T> (SO) /
cycloalkenyl<(3-8)> (SO) / aryl<(6-12)> (SO) /
heteroaryl<EC (-12) A (1-) Q> (SO) / 64 / 47



G14 = NULL / alkylene<(1-8)> / alkenylene<(2-8)>
G15 = 66-15 67-51 / 60-15 61-51 / 52-15 53-51 /
69-15 71-51 / 72-15 74-51

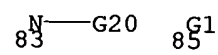


G16 = 54-15 55-53 / 56-15 57-53 / 77-15 79-53

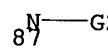


G17 = alkylene<(1-8)> / alkenylene<(2-8)>
G18 = Ak<EC (1-8) C, BD (0-) D (0-) T> (SO) /
Cb<EC (3-8) C, BD (0-) D (0) T> (SO) /
Hy<EC (3-8) A (1-) Q, AR (0), BD (0-) D (0) T> (SO)
G19 = NH / 75

G20 = alkyl<(1-8)>
G21 = O / NH / 83 / 85-15 86-81

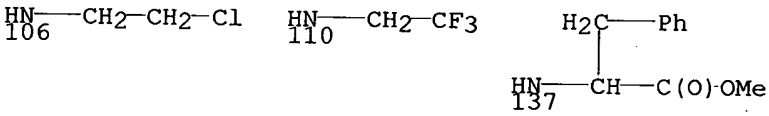


G22 = O / NH / 87



G23 = H / OH
G24 = OH / alkoxy<(1-8)> / NH2 / F / Cl / Br / I / SO3H / OSO3H / 143 / alkylcarbonyloxy<(1-8)> / alkylcarbonylamino<(1-8)> / alkylcarbonyl<(1-8)> / alkylsulfinyl<(1-8)> / alkylsulfonyl<(1-8)> / alkylthio<(1-8)>

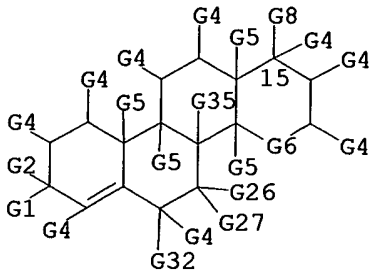
G25 = OMe / 106 / 110 / 137



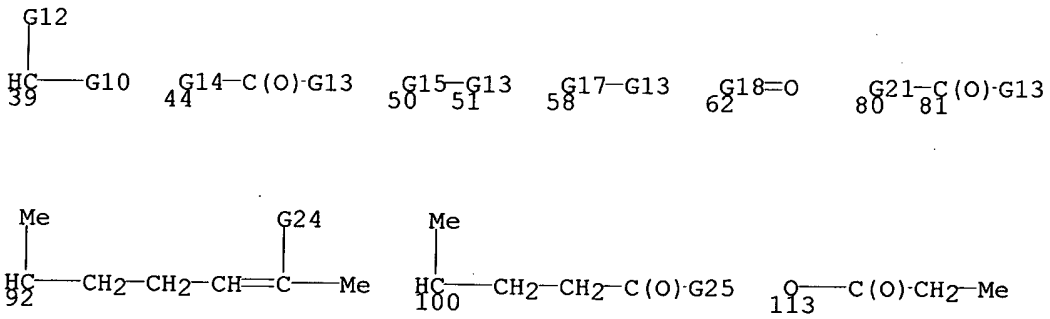
G26 = H / OH / NH2 / CO2H / F / Cl / Br / I / SO3H / OSO3H / alkyl<(1-8)> (SO (1-) G3)
G27 = H
G28 = OH / alkoxy<(1-8)> / alkylamino<(1-8)> / OEt
G29 = F / OH / H
G30 = H / OH / NH2 / CO2H / F / Cl / Br / I / SO3H / OSO3H / alkyl<(1-8)> (SO (1-) G3)
G31 = H / alkyl<(1-8)> (SO (1-) G7) / alkyl<(1-8)> (SR (1-) OH) / alkoxy<(1-8)> / OH / NH2 / (SC Me)
G32 = H
G33 = CF3 / OSO3H / CO2H / CONH2
G34 = H / F
G35 = H / alkyl<(1-8)> (SO (1-) G7) / alkyl<(1-8)> (SR (1-) OH) / alkoxy<(1-8)> / OH / NH2 / (SC Me)
G1 +G2 = O
G26+G27= O
G27+G35= NULL
MPL: claim 1

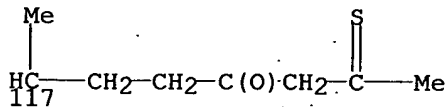
NTE: additional derivatization also claimed
NTE: substitution is restricted
NTE: or salts
NTE: also incorporates claims 18, 35 and 49

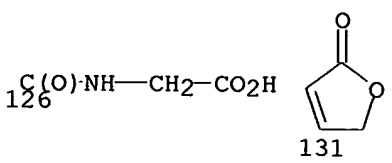
MSTR 1B

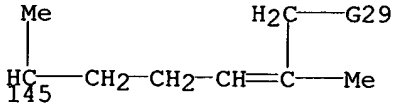


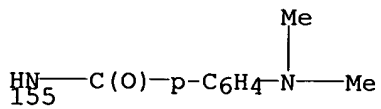
G1 = H / OH / NH2 / CO2H / F / Cl / Br / I / SO3H / OSO3H / alkyl<(1-8)> (SO (1-) G3)
G2 = H
G3 = OH / F / Cl / Br / I / NH2 / **CO2H** / SO3H / OSO3H
G4 = H / **OH** / NH2 / CO2H / F / Cl / Br / I / SO3H / OSO3H / alkyl<(1-8)> (SO (1-) G3)
G5 = H / alkyl<(1-8)> (SO (1-) G7) / alkyl<(1-8)> (SR (1-) OH) / alkoxy<(1-8)> / OH / NH2 / **(SC Me)**
G6 = (0-2) CH2
G7 = F / Cl / Br / I
G8 = alkyl<(1-8)> (SO (1-) G9) / alkenyl<(2-8)> (SO) / alkynyl<(2-8)> (SO) / cycloalkyl<(3-8)> (SO) / Hy<EC (3-8) A (1-) Q, AR (0), BD (0-) D (0) T> (SO) / cycloalkenyl<(3-8)> (SO) / aryl<(6-12)> (SO) / heteroaryl<EC (-12) A (1-) Q> (SO) / 62 / **39** / 58 / 44 / 50 / 80 / (SC 92 / 100 / 113 / 117 / 126 / 131 / 145 / 155 / 161 / 169 / 183)

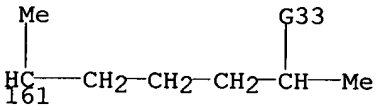


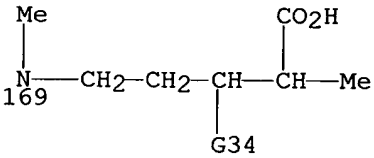


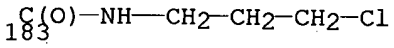




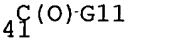




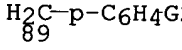




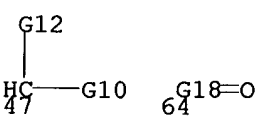
G9 = R / aryl<(6-12)> (SO) /
heteroaryl<EC (-12) A (1-) Q> (SO)
G10 = H / NH2 / alkylamino<(1-8)> / dialkylamino<(1-8)> /
41



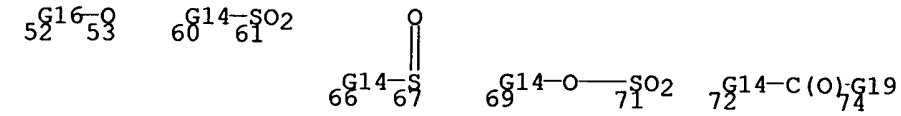
G11 = OH / alkoxy<(1-8)>
G12 = H / R<TX "side chain of amino acid"> / (SC 89)



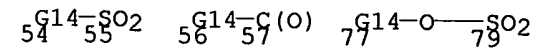
G13 = alkyl<(1-8)> (SO (1-) G9) / alkenyl<(2-8)> (SO) /
alkynyl<(2-8)> (SO) / cycloalkyl<(3-8)> (SO) /
Hy<EC (3-8) A (1-) Q, AR (0), BD (0-) D (0) T> (SO) /
cycloalkenyl<(3-8)> (SO) / aryl<(6-12)> (SO) /
heteroaryl<EC (-12) A (1-) Q> (SO) / 64 / 47



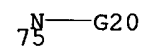
G14 = NULL / alkylene<(1-8)> / alkenylene<(2-8)>
G15 = 66-15 67-51 / 60-15 61-51 / 52-15 53-51 /
69-15 71-51 / 72-15 74-51



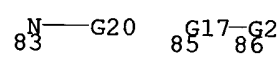
G16 = 54-15 55-53 / 56-15 57-53 / 77-15 79-53



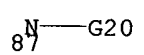
G17 = alkylene<(1-8)> / alkenylene<(2-8)>
G18 = Ak<EC (1-8) C, BD (0-) D (0-) T> (SO) /
Cb<EC (3-8) C, BD (0-) D (0) T> (SO) /
Hy<EC (3-8) A (1-) Q, AR (0), BD (0-) D (0) T> (SO)
G19 = NH / 75



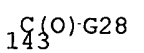
G20 = alkyl<(1-8)>
G21 = O / NH / 83 / 85-15 86-81



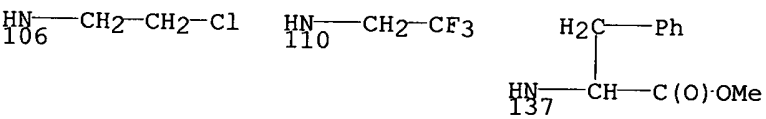
G22 = O / NH / 87



G23 = H / OH
G24 = OH / alkoxy<(1-8)> / NH2 / F / Cl / Br / I / SO3H /
OSO3H / 143 / alkylcarbonyloxy<(1-8)> /
alkylcarbonylamino<(1-8)> / alkylcarbonyl<(1-8)> /
alkylsulfinyl<(1-8)> / alkylsulfonyl<(1-8)> /
alkylthio<(1-8)>

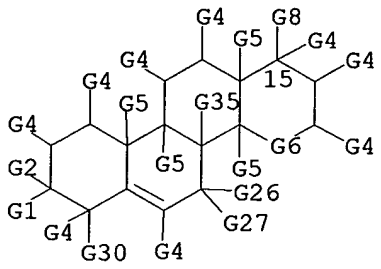


G25 = OMe / 106 / 110 / 137

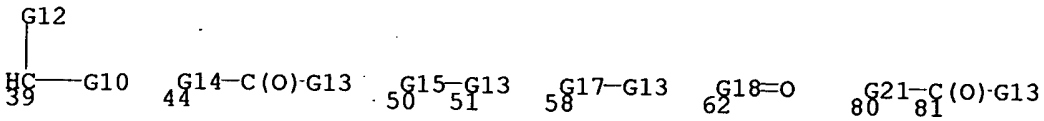


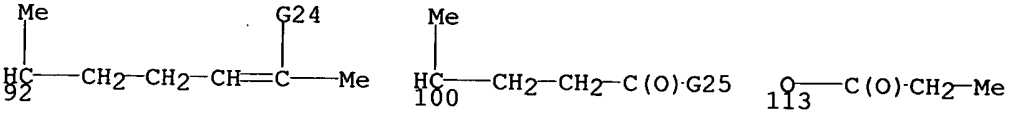
G26 = H / OH / NH2 / CO2H / F / Cl / Br / I / SO3H / OSO3H / **alkyl<(1-8)> (SO (1-) G3)**
G27 = H
G28 = OH / alkoxy<(1-8)> / alkylamino<(1-8)> / OEt
G29 = F / OH / H
G32 = H
G33 = CF3 / OSO3H / CO2H / CONH2
G34 = H / F
G35 = H / alkyl<(1-8)> (SO (1-) G7) / alkyl<(1-8)> (SR (1-) OH) / alkoxy<(1-8)> / OH / NH2 / (SC Me)
G1 +G2 = **O**
G26+G27= O
G27+G35= NULL
MPL: claim 1
NTE: additional derivatization also claimed
NTE: substitution is restricted
NTE: or salts
NTE: also incorporates claims 18, 35 and 49

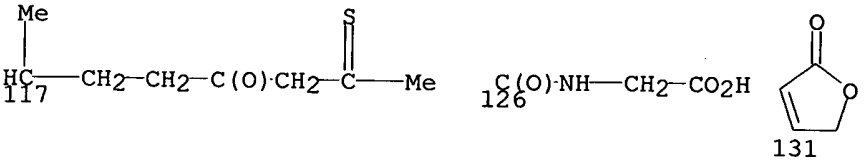
MSTR 1C

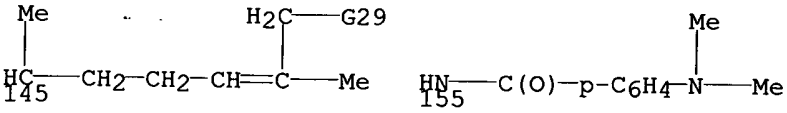


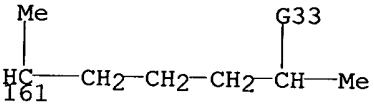
G1 = H / OH / NH2 / CO2H / F / Cl / Br / I / SO3H / OSO3H / alkyl<(1-8)> (SO (1-) G3)
G2 = H
G3 = OH / F / Cl / Br / I / NH2 / CO2H / SO3H / OSO3H
G4 = H / OH / NH2 / CO2H / F / Cl / Br / I / SO3H / OSO3H / alkyl<(1-8)> (SO (1-) G3)
G5 = H / alkyl<(1-8)> (SO (1-) G7) / alkyl<(1-8)> (SR (1-) OH) / alkoxy<(1-8)> / OH / NH2 / (SC Me)
G6 = (0-2) CH2
G7 = F / Cl / Br / I
G8 = alkyl<(1-8)> (SO (1-) G9) / alkenyl<(2-8)> (SO) / alkynyl<(2-8)> (SO) / cycloalkyl<(3-8)> (SO) / Hy<EC (3-8) A (1-) Q, AR (0), BD (0-) D (0) T> (SO) / cycloalkenyl<(3-8)> (SO) / aryl<(6-12)> (SO) / heteroaryl<EC (-12) A (1-) Q> (SO) / 62 / 39 / 58 / 44 / 50 / 80 / (SC 92 / 100 / 113 / 117 / 126 / 131 / 145 / 155 / 161 / 169 / 183)

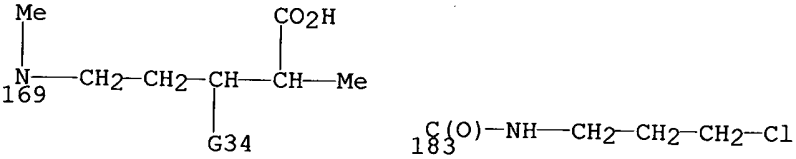




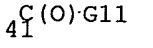




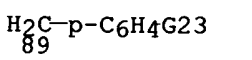




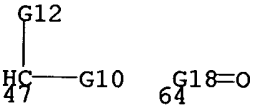
G9 = R / aryl<(6-12)> (SO) /
heteroaryl<EC (-12) A (1-) Q> (SO)
G10 = H / NH2 / alkylamino<(1-8)> / dialkylamino<(1-8)> /
41



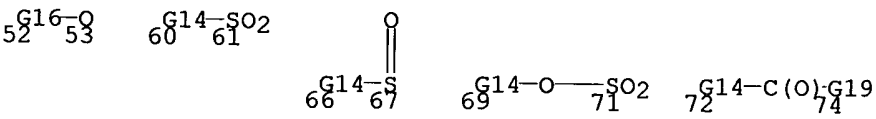
G11 = OH / alkoxy<(1-8)>
G12 = H / R<TX "side chain of amino acid"> / (SC 89)



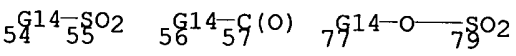
G13 = alkyl<(1-8)> (SO (1-) G9) / alkenyl<(2-8)> (SO) /
alkynyl<(2-8)> (SO) / cycloalkyl<(3-8)> (SO) /
Hy<EC (3-8) A (1-) Q, AR (0), BD (0-) D (0) T> (SO) /
cycloalkenyl<(3-8)> (SO) / aryl<(6-12)> (SO) /
heteroaryl<EC (-12) A (1-) Q> (SO) / 64 / 47



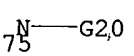
G14 = NULL / alkylene<(1-8)> / alkenylene<(2-8)>
G15 = 66-15 67-51 / 60-15 61-51 / 52-15 53-51 /
69-15 71-51 / 72-15 74-51



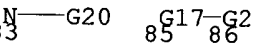
G16 = 54-15 55-53 / 56-15 57-53 / 77-15 79-53



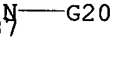
G17 = alkylene<(1-8)> / alkenylene<(2-8)>
G18 = Ak<EC (1-8) C, BD (0-) D (0-) T> (SO) /
Cb<EC (3-8) C, BD (0-) D (0) T> (SO) /
Hy<EC (3-8) A (1-) Q, AR (0), BD (0-) D (0) T> (SO)
G19 = NH / 75



G20 = alkyl<(1-8)>
G21 = O / NH / 83 / 85-15 86-81

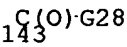


G22 = O / NH / 87

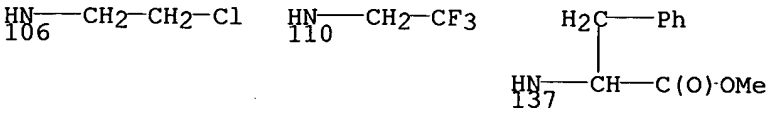


G23 = H / OH
G24 = OH / alkoxy<(1-8)> / NH2 / F / Cl / Br / I / SO3H /

OSO3H / 143 / alkylcarbonyloxy<(1-8)> /
alkylcarbonylamino<(1-8)> / alkylcarbonyl<(1-8)> /
alkylsulfinyl<(1-8)> / alkylsulfonyl<(1-8)> /
alkylthio<(1-8)>



G25 = OMe / 106 / 110 / 137



G26 = H / OH / NH2 / CO2H / F / Cl / Br / I / SO3H /
OSO3H / alkyl<(1-8)> (SO (1-) G3)
G27 = H
G28 = OH / alkoxy<(1-8)> / alkylamino<(1-8)> / OEt
G29 = F / OH / H
G30 = H / OH / NH2 / CO2H / F / Cl / Br / I / SO3H /
OSO3H / alkyl<(1-8)> (SO (1-) G3)
G33 = CF3 / OSO3H / CO2H / CONH2
G34 = H / F
G35 = H / alkyl<(1-8)> (SO (1-) G7) /
alkyl<(1-8)> (SR (1-) OH) / alkoxy<(1-8)> / OH / NH2 /
(SC Me)
G1 +G2 = O
G26+G27= O
G27+G35= NULL
MPL: claim 1
NTE: additional derivatization also claimed
NTE: substitution is restricted
NTE: or salts
NTE: also incorporates claims 18, 35 and 49